



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:04 AM UTC

PDB ID : 6PM9 / pdb_00006pm9
Title : Crystal structure of the core catalytic domain of human O-GlcNAcase bound to MK-8719
Authors : Klein, D.J.; Selnick, H.G.; Duffy, J.L.; McEachern, E.J.
Deposited on : 2019-07-01
Resolution : 2.86 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:

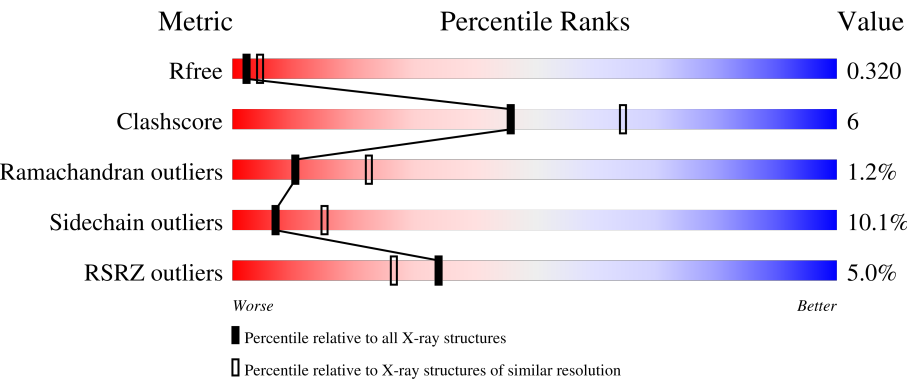
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	388	2% 59%17%•20%
1	B	388	2% 62%16%•20%
1	C	388	2% 55%21%•20%
1	D	388	2% 58%19%•20%
2	E	161	11% 48%20%•30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	161	7%51%12%. .32%
2	G	161	6%53%16%.27%
2	H	161	14%48%19%..30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13916 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 O-GlcNAcase TIM-barrel domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2540	1644	418	464	14			
1	B	309	Total	C	N	O	S	0	0	0
			2536	1641	417	464	14			
1	C	310	Total	C	N	O	S	0	0	0
			2515	1626	416	459	14			
1	D	310	Total	C	N	O	S	0	0	0
			2512	1624	414	460	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP O60502
B	13	GLY	-	expression tag	UNP O60502
C	13	GLY	-	expression tag	UNP O60502
D	13	GLY	-	expression tag	UNP O60502

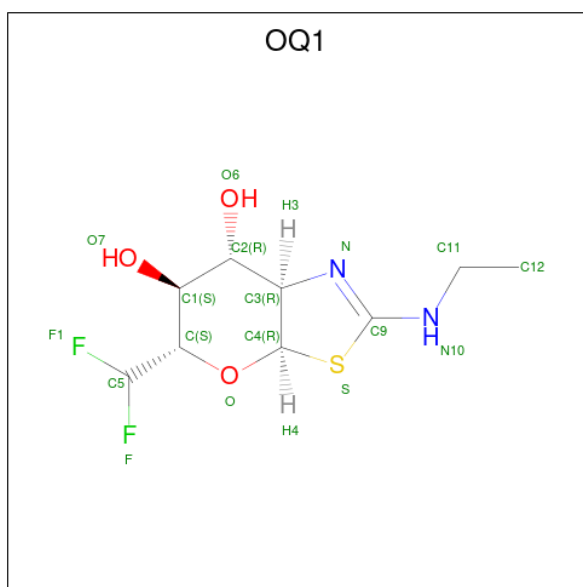
- Molecule 2 is a protein called O-GlcNAcase stalk domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	112	Total	C	N	O	S	0	0	0
			912	588	152	163	9			
2	F	109	Total	C	N	O	S	0	0	0
			896	580	149	158	9			
2	G	117	Total	C	N	O	S	0	0	0
			974	631	163	171	9			
2	H	112	Total	C	N	O	S	0	0	0
			928	600	156	163	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	553	MET	-	initiating methionine	UNP O60502
E	706	HIS	-	expression tag	UNP O60502
E	707	HIS	-	expression tag	UNP O60502
E	708	HIS	-	expression tag	UNP O60502
E	709	HIS	-	expression tag	UNP O60502
E	710	HIS	-	expression tag	UNP O60502
E	711	HIS	-	expression tag	UNP O60502
E	712	HIS	-	expression tag	UNP O60502
E	713	HIS	-	expression tag	UNP O60502
F	553	MET	-	initiating methionine	UNP O60502
F	706	HIS	-	expression tag	UNP O60502
F	707	HIS	-	expression tag	UNP O60502
F	708	HIS	-	expression tag	UNP O60502
F	709	HIS	-	expression tag	UNP O60502
F	710	HIS	-	expression tag	UNP O60502
F	711	HIS	-	expression tag	UNP O60502
F	712	HIS	-	expression tag	UNP O60502
F	713	HIS	-	expression tag	UNP O60502
G	553	MET	-	initiating methionine	UNP O60502
G	706	HIS	-	expression tag	UNP O60502
G	707	HIS	-	expression tag	UNP O60502
G	708	HIS	-	expression tag	UNP O60502
G	709	HIS	-	expression tag	UNP O60502
G	710	HIS	-	expression tag	UNP O60502
G	711	HIS	-	expression tag	UNP O60502
G	712	HIS	-	expression tag	UNP O60502
G	713	HIS	-	expression tag	UNP O60502
H	553	MET	-	initiating methionine	UNP O60502
H	706	HIS	-	expression tag	UNP O60502
H	707	HIS	-	expression tag	UNP O60502
H	708	HIS	-	expression tag	UNP O60502
H	709	HIS	-	expression tag	UNP O60502
H	710	HIS	-	expression tag	UNP O60502
H	711	HIS	-	expression tag	UNP O60502
H	712	HIS	-	expression tag	UNP O60502
H	713	HIS	-	expression tag	UNP O60502

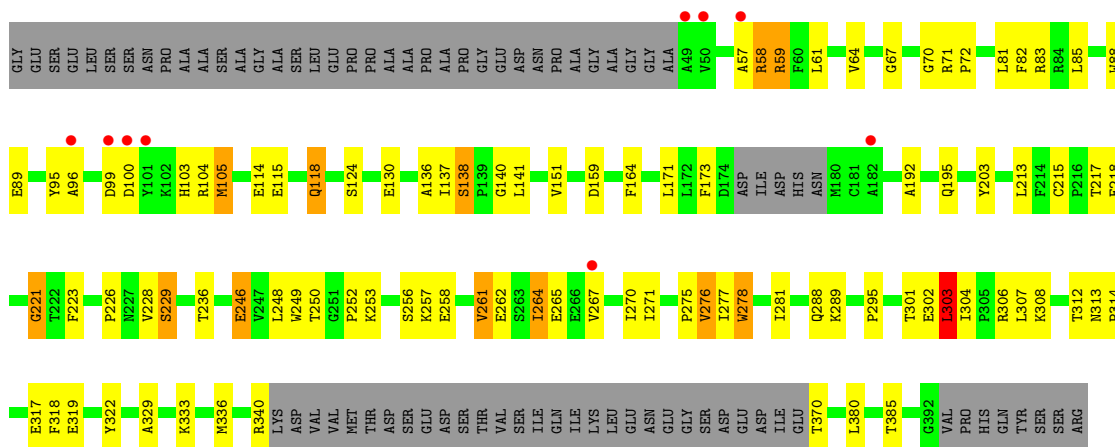
- Molecule 3 is (3aR,5S,6S,7R,7aR)-5-(difluoromethyl)-2-(ethylamino)-5,6,7,7a-tetrahydro-3aH-pyrano[3,2-d][1,3]thiazole-6,7-diol (CCD ID: OQ1) (formula: C₉H₁₄F₂N₂O₃S) (labeled as "Ligand of Interest" by depositor).



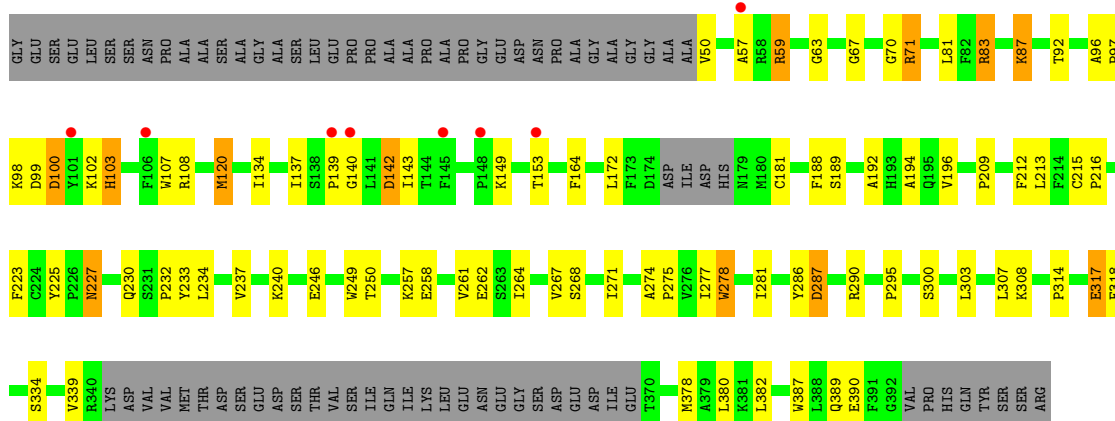
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			17	9	2	2	3	1		
3	B	1	Total	C	F	N	O	S	0	0
			17	9	2	2	3	1		
3	C	1	Total	C	F	N	O	S	0	0
			17	9	2	2	3	1		
3	D	1	Total	C	F	N	O	S	0	0
			17	9	2	2	3	1		

- Molecule 4 is water.

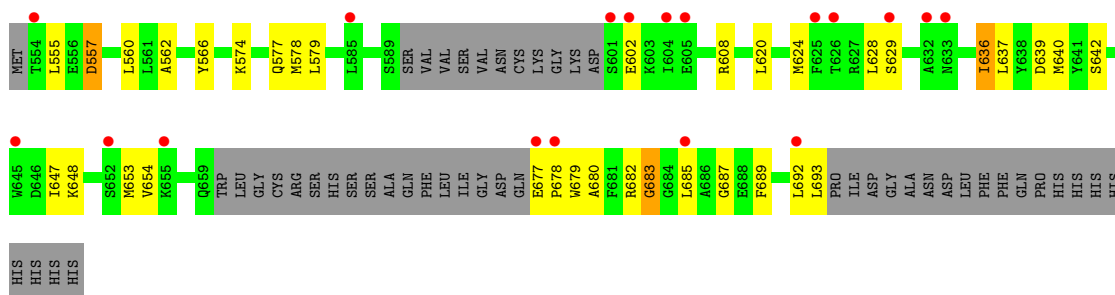
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	9	Total	O	0	0
			9	9		
4	C	8	Total	O	0	0
			8	8		
4	D	3	Total	O	0	0
			3	3		
4	E	2	Total	O	0	0
			2	2		
4	F	3	Total	O	0	0
			3	3		
4	G	1	Total	O	0	0
			1	1		
4	H	3	Total	O	0	0
			3	3		



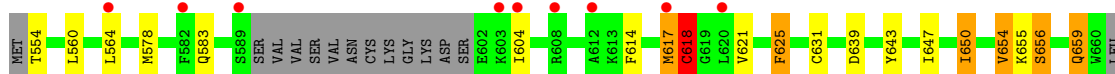
- Molecule 1: O-GlcNAcase TIM-barrel domain



- Molecule 2: O-GlcNAcase stalk domain

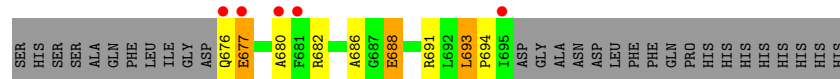


- Molecule 2: O-GlcNAcase stalk domain

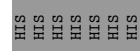
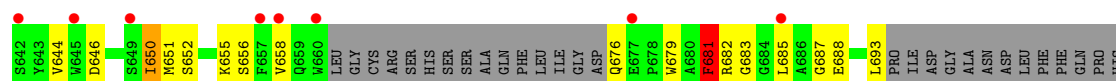
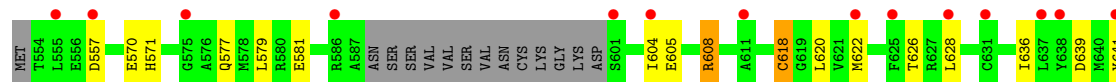




• Molecule 2: O-GlcNAcase stalk domain



• Molecule 2: O-GlcNAcase stalk domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	89.92Å 91.46Å 94.61Å 77.27° 62.61° 62.86°	Depositor
Resolution (Å)	40.69 – 2.86 40.69 – 2.86	Depositor EDS
% Data completeness (in resolution range)	95.1 (40.69-2.86) 95.0 (40.69-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.239 , 0.309 0.251 , 0.320	Depositor DCC
R_{free} test set	2706 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 80.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,l,h-k 0.000 for h,h-l,k 0.000 for h,h-k,h-l 0.000 for -h,-h+k,-l 0.000 for -h,-k,-h+l 0.000 for -h,-l,-k 0.000 for -h,-h+l,-h+k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13916	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7595e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: OQ1

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	0.86	0/2610	1.45	30/3539 (0.8%)
1	B	0.88	0/2606	1.48	25/3535 (0.7%)
1	C	0.92	0/2580	1.47	21/3494 (0.6%)
1	D	0.88	0/2577	1.44	17/3491 (0.5%)
2	E	0.84	0/932	1.50	12/1251 (1.0%)
2	F	0.86	0/916	1.57	10/1230 (0.8%)
2	G	0.90	1/998 (0.1%)	1.54	17/1341 (1.3%)
2	H	0.81	0/950	1.48	7/1276 (0.5%)
All	All	0.88	1/14169 (0.0%)	1.48	139/19157 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	677	GLU	CA-C	5.24	1.59	1.52

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	ASP	CA-CB-CG	9.81	122.41	112.60
2	H	605	GLU	N-CA-C	-9.20	102.19	113.41
1	B	140	GLY	N-CA-C	7.86	123.72	113.27
2	F	654	VAL	N-CA-C	-7.71	103.28	110.53
1	A	186	GLU	CA-C-N	7.46	129.96	120.56
1	A	186	GLU	C-N-CA	7.46	129.96	120.56
1	B	159	ASP	CA-CB-CG	7.19	119.79	112.60
2	E	683	GLY	N-CA-C	6.81	121.76	113.79
1	C	217	THR	N-CA-C	-6.76	103.37	111.69
2	G	652	SER	N-CA-C	-6.75	103.16	111.40
1	B	164	PHE	CA-CB-CG	6.64	120.44	113.80
1	C	261	VAL	CA-C-N	6.52	129.35	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	261	VAL	C-N-CA	6.52	129.35	120.54
2	E	557	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	302	GLU	CA-C-N	6.43	129.42	120.29
1	A	302	GLU	C-N-CA	6.43	129.42	120.29
2	E	562	ALA	CA-C-N	6.38	129.12	120.38
2	E	562	ALA	C-N-CA	6.38	129.12	120.38
1	B	303	LEU	CA-C-N	6.37	125.42	120.33
1	B	303	LEU	C-N-CA	6.37	125.42	120.33
1	B	127	ARG	CA-C-N	6.30	128.72	120.28
1	B	127	ARG	C-N-CA	6.30	128.72	120.28
1	C	164	PHE	CA-CB-CG	6.22	120.02	113.80
1	D	287	ASP	CA-C-N	6.20	128.50	120.44
1	D	287	ASP	C-N-CA	6.20	128.50	120.44
1	B	201	GLU	CA-C-N	6.16	128.40	120.70
1	B	201	GLU	C-N-CA	6.16	128.40	120.70
2	G	654	VAL	N-CA-C	-6.15	104.85	110.82
2	H	571	HIS	N-CA-C	-6.11	100.61	110.32
1	A	195	GLN	CA-C-N	6.08	128.78	120.46
1	A	195	GLN	C-N-CA	6.08	128.78	120.46
1	B	376	PRO	CA-C-N	5.88	128.08	120.44
1	B	376	PRO	C-N-CA	5.88	128.08	120.44
1	D	194	ALA	CA-C-N	5.87	128.14	120.28
1	D	194	ALA	C-N-CA	5.87	128.14	120.28
2	E	648	LYS	CA-C-N	5.85	128.39	120.38
2	E	648	LYS	C-N-CA	5.85	128.39	120.38
1	D	268	SER	CA-C-N	5.83	128.37	120.44
1	D	268	SER	C-N-CA	5.83	128.37	120.44
1	A	236	THR	CA-C-N	5.83	128.11	120.60
1	A	236	THR	C-N-CA	5.83	128.11	120.60
1	A	284	ASN	CA-CB-CG	5.83	118.42	112.60
2	G	577	GLN	CA-C-N	5.81	128.00	120.44
2	G	577	GLN	C-N-CA	5.81	128.00	120.44
1	A	174	ASP	CA-CB-CG	5.80	118.40	112.60
1	C	203	TYR	N-CA-C	-5.76	104.69	110.97
1	A	80	GLU	CB-CG-CD	5.76	122.39	112.60
1	A	100	ASP	CA-CB-CG	5.74	118.34	112.60
1	C	226	PRO	CA-C-N	5.74	129.73	122.16
1	C	226	PRO	C-N-CA	5.74	129.73	122.16
1	C	276	VAL	N-CA-C	-5.72	100.18	108.36
1	B	126	ALA	CA-C-N	5.71	128.20	120.38
1	B	126	ALA	C-N-CA	5.71	128.20	120.38
1	B	337	ASN	CA-C-N	5.70	125.39	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	ASN	C-N-CA	5.70	125.39	119.92
1	A	116	ALA	CA-C-N	5.69	128.22	120.54
1	A	116	ALA	C-N-CA	5.69	128.22	120.54
1	B	174	ASP	CA-C-N	-5.69	115.16	122.79
1	B	174	ASP	C-N-CA	-5.69	115.16	122.79
1	C	304	ILE	N-CA-CB	5.65	114.31	110.52
1	D	216	PRO	CA-C-N	5.62	127.75	120.44
1	D	216	PRO	C-N-CA	5.62	127.75	120.44
2	H	618	CYS	N-CA-C	-5.62	104.55	111.40
1	A	124	SER	CA-C-N	5.62	128.07	120.38
1	A	124	SER	C-N-CA	5.62	128.07	120.38
1	B	139	PRO	CA-C-N	5.60	127.18	120.13
1	B	139	PRO	C-N-CA	5.60	127.18	120.13
1	A	265	GLU	CA-C-N	5.58	128.22	120.29
1	A	265	GLU	C-N-CA	5.58	128.22	120.29
1	A	182	ALA	CA-C-N	5.57	128.01	120.38
1	A	182	ALA	C-N-CA	5.57	128.01	120.38
1	B	142	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	164	PHE	CA-CB-CG	5.55	119.35	113.80
2	G	602	GLU	CA-C-N	5.53	130.25	121.18
2	G	602	GLU	C-N-CA	5.53	130.25	121.18
1	A	303	LEU	CA-C-N	5.50	125.71	120.43
1	A	303	LEU	C-N-CA	5.50	125.71	120.43
2	F	625	PHE	CA-CB-CG	5.50	119.30	113.80
2	G	677	GLU	N-CA-C	5.47	121.91	109.81
2	F	618	CYS	CA-C-N	5.43	125.97	120.00
2	F	618	CYS	C-N-CA	5.43	125.97	120.00
1	B	276	VAL	N-CA-C	-5.42	100.58	108.17
1	D	100	ASP	N-CA-C	-5.40	102.05	110.42
2	G	636	ILE	CA-C-N	5.40	127.46	120.44
2	G	636	ILE	C-N-CA	5.40	127.46	120.44
1	D	188	PHE	CA-C-N	5.38	128.03	120.28
1	D	188	PHE	C-N-CA	5.38	128.03	120.28
1	C	159	ASP	CA-C-N	5.34	127.43	120.28
1	C	159	ASP	C-N-CA	5.34	127.43	120.28
1	D	262	GLU	CA-C-N	5.34	127.38	120.44
1	D	262	GLU	C-N-CA	5.34	127.38	120.44
1	C	221	GLY	CA-C-N	5.33	128.17	120.38
1	C	221	GLY	C-N-CA	5.33	128.17	120.38
1	C	303	LEU	CA-C-N	5.33	125.55	120.43
1	C	303	LEU	C-N-CA	5.33	125.55	120.43
2	H	682	ARG	N-CA-C	5.32	117.73	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	555	LEU	CA-C-N	5.31	128.13	120.38
2	E	555	LEU	C-N-CA	5.31	128.13	120.38
1	C	265	GLU	CA-C-N	5.27	127.60	120.44
1	C	265	GLU	C-N-CA	5.27	127.60	120.44
1	C	257	LYS	N-CA-C	-5.26	105.46	111.14
1	C	82	PHE	CA-CB-CG	5.26	119.06	113.80
2	G	623	GLY	CA-C-N	5.25	127.32	120.28
2	G	623	GLY	C-N-CA	5.25	127.32	120.28
1	A	317	GLU	CA-C-N	5.24	127.56	120.38
1	A	317	GLU	C-N-CA	5.24	127.56	120.38
1	A	217	THR	N-CA-C	-5.24	105.25	111.69
1	A	228	VAL	CA-C-N	5.23	127.24	120.44
1	A	228	VAL	C-N-CA	5.23	127.24	120.44
2	G	677	GLU	CA-C-O	-5.22	113.01	120.16
1	B	100	ASP	N-CA-C	-5.22	98.05	107.75
1	D	387	TRP	CA-C-N	5.21	127.52	120.38
1	D	387	TRP	C-N-CA	5.21	127.52	120.38
2	G	686	ALA	CA-C-N	5.21	125.74	120.00
2	G	686	ALA	C-N-CA	5.21	125.74	120.00
2	F	687	GLY	CA-C-N	5.20	127.50	120.38
2	F	687	GLY	C-N-CA	5.20	127.50	120.38
1	D	223	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	106	PHE	CA-CB-CG	5.17	118.97	113.80
2	H	652	SER	CA-C-N	5.15	127.18	120.28
2	H	652	SER	C-N-CA	5.15	127.18	120.28
2	G	555	LEU	CA-C-N	5.13	127.87	120.38
2	G	555	LEU	C-N-CA	5.13	127.87	120.38
1	B	371	ASP	CA-C-N	5.12	129.10	120.29
1	B	371	ASP	C-N-CA	5.12	129.10	120.29
1	C	159	ASP	CA-CB-CG	5.11	117.71	112.60
2	F	614	PHE	CA-C-N	5.09	127.61	120.28
2	F	614	PHE	C-N-CA	5.09	127.61	120.28
1	D	389	GLN	CB-CG-CD	5.08	121.24	112.60
2	H	557	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	278	TRP	N-CA-C	-5.05	98.64	107.73
2	E	578	MET	CA-C-N	5.04	127.04	120.28
2	E	578	MET	C-N-CA	5.04	127.04	120.28
2	F	617	MET	CA-C-N	5.04	126.99	120.44
2	F	617	MET	C-N-CA	5.04	126.99	120.44
1	C	278	TRP	N-CA-C	-5.02	98.41	107.75
2	E	642	SER	CA-C-N	5.01	127.70	120.38
2	E	642	SER	C-N-CA	5.01	127.70	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	588	ASN	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2540	0	2484	32	0
1	B	2536	0	2473	18	0
1	C	2515	0	2474	35	0
1	D	2512	0	2464	39	0
2	E	912	0	887	9	0
2	F	896	0	880	11	0
2	G	974	0	953	12	0
2	H	928	0	905	15	0
3	A	17	0	0	1	0
3	B	17	0	0	0	0
3	C	17	0	0	0	0
3	D	17	0	0	1	0
4	A	6	0	0	0	0
4	B	9	0	0	0	0
4	C	8	0	0	0	0
4	D	3	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
4	G	1	0	0	0	0
4	H	3	0	0	0	0
All	All	13916	0	13520	158	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 6.

All (158) 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:D:264:ILE:HD11	1:D:303:LEU:HG	1.61	0.82
1:D:71:ARG:HE	2:H:641:TYR:HD2	1.24	0.82
1:B:97:PRO:HB2	1:B:100:ASP:HB2	1.62	0.80
1:C:64:VAL:HG23	1:C:85:LEU:HD21	1.64	0.78
1:C:218:GLU:HG2	1:C:223:PHE:O	1.94	0.67
1:B:248:LEU:HD22	1:B:278:TRP:HD1	1.62	0.64
1:A:78:ARG:HB3	1:A:122:LEU:HD11	1.80	0.63
1:D:70:GLY:H	1:D:99:ASP:HB2	1.64	0.63
1:D:264:ILE:CD1	1:D:303:LEU:HG	2.28	0.63
1:C:104:ARG:HG3	1:C:138:SER:HB2	1.80	0.62
1:D:71:ARG:NE	2:H:641:TYR:HD2	1.96	0.61
2:E:683:GLY:HA3	2:E:687:GLY:HA3	1.85	0.58
1:B:248:LEU:HD22	1:B:278:TRP:CD1	2.39	0.58
1:C:58:ARG:O	1:C:59:ARG:HG3	2.05	0.57
2:F:578:MET:HE3	2:F:617:MET:HG3	1.86	0.57
1:D:108:ARG:HH12	1:D:142:ASP:HB2	1.70	0.56
2:E:557:ASP:HB3	2:E:624:MET:HG2	1.86	0.56
1:D:172:LEU:HD23	1:D:215:CYS:CB	2.34	0.56
1:D:227:ASN:HD21	1:D:230:GLN:HB2	1.71	0.56
2:E:692:LEU:HD23	2:G:583:GLN:HE21	1.70	0.56
1:D:295:PRO:HD3	1:D:380:LEU:HD22	1.88	0.55
1:C:295:PRO:HD3	1:C:380:LEU:HD22	1.89	0.55
1:A:253:LYS:HE3	1:A:256:SER:HA	1.89	0.55
1:D:250:THR:HG22	1:D:278:TRP:O	2.08	0.54
1:A:83:ARG:HG2	1:A:129:TYR:CZ	2.43	0.54
1:C:81:LEU:HB2	1:C:318:PHE:HE1	1.73	0.54
1:B:192:ALA:HB2	1:B:233:TYR:CD1	2.44	0.53
1:C:301:THR:C	1:C:303:LEU:H	2.16	0.53
2:E:689:PHE:CE2	2:H:651:MET:HE1	2.44	0.53
2:H:577:GLN:O	2:H:581:GLU:HG2	2.09	0.53
2:F:656:SER:HA	2:F:659:GLN:HG3	1.91	0.52
1:B:67:GLY:HA2	1:B:96:ALA:O	2.09	0.52
1:A:241:LEU:HD23	1:A:273:ARG:NH2	2.24	0.52
1:C:295:PRO:HB3	1:C:380:LEU:HB2	1.92	0.52
1:D:209:PRO:HG2	1:D:212:PHE:HB2	1.93	0.51
1:D:192:ALA:HB2	1:D:233:TYR:CD1	2.45	0.51
1:B:296:TYR:CZ	1:B:299:ARG:HD3	2.45	0.51
2:F:617:MET:O	2:F:621:VAL:HG23	2.10	0.51
1:C:95:TYR:O	1:C:136:ALA:HB3	2.11	0.51
2:F:690:GLN:HA	2:F:693:LEU:HD12	1.93	0.51
1:C:173:PHE:HB3	1:C:195:GLN:HE21	1.75	0.51
1:D:172:LEU:HD23	1:D:215:CYS:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:VAL:O	1:D:271:ILE:HG12	2.11	0.51
1:A:263:SER:O	1:A:267:VAL:HG23	2.12	0.50
1:C:115:GLU:O	1:C:118:GLN:HG2	2.11	0.50
1:D:317:GLU:HB2	2:E:639:ASP:HB3	1.93	0.49
1:B:297:LYS:HG3	1:B:376:PRO:HG3	1.94	0.49
1:D:300:SER:O	1:D:303:LEU:HB2	2.12	0.49
1:D:249:TRP:O	1:D:277:ILE:HA	2.12	0.49
2:G:617:MET:SD	2:G:620:LEU:HD23	2.52	0.49
1:C:267:VAL:O	1:C:271:ILE:HG12	2.12	0.49
1:A:97:PRO:HB2	1:A:100:ASP:HB3	1.93	0.49
1:C:312:THR:O	1:C:314:PRO:HD3	2.13	0.49
2:G:650:ILE:O	2:G:654:VAL:HG23	2.13	0.49
1:B:339:VAL:HG23	1:B:340:ARG:H	1.78	0.49
1:A:104:ARG:HG3	1:A:138:SER:HB2	1.95	0.49
2:F:694:PRO:C	2:F:695:ILE:HG13	2.38	0.49
1:B:234:LEU:HB3	1:B:270:ILE:HG12	1.95	0.49
2:G:560:LEU:HD21	2:G:621:VAL:HA	1.95	0.48
2:H:622:MET:HE1	2:H:655:LYS:HD3	1.95	0.48
1:C:252:PRO:HD2	1:C:256:SER:OG	2.14	0.48
2:E:653:MET:HE2	2:H:693:LEU:HD13	1.96	0.48
1:C:276:VAL:HG22	1:C:308:LYS:HB2	1.96	0.48
1:D:107:TRP:CE2	1:D:139:PRO:HB3	2.49	0.48
1:B:145:PHE:CG	1:B:194:ALA:HB1	2.49	0.48
1:C:264:ILE:HD11	1:C:306:ARG:HB3	1.95	0.48
1:D:196:VAL:HG11	1:D:240:LYS:HB2	1.95	0.48
1:A:264:ILE:HD11	1:A:306:ARG:HB3	1.95	0.47
1:D:59:ARG:O	1:D:59:ARG:HG2	2.12	0.47
1:D:274:ALA:HB3	1:D:308:LYS:HG2	1.96	0.47
1:A:284:ASN:HD22	1:A:291:LEU:HA	1.80	0.47
1:A:296:TYR:CZ	1:A:299:ARG:HD3	2.50	0.47
1:D:287:ASP:HB3	1:D:290:ARG:HB2	1.96	0.47
2:F:560:LEU:O	2:F:564:LEU:HG	2.15	0.47
1:A:172:LEU:HA	1:A:215:CYS:HB3	1.97	0.47
1:B:196:VAL:HG11	1:B:240:LYS:HB2	1.97	0.47
1:C:250:THR:HG22	1:C:278:TRP:O	2.15	0.47
1:C:319:GLU:HB3	2:H:636:ILE:HG23	1.97	0.47
1:D:277:ILE:HG12	1:D:307:LEU:HD22	1.96	0.47
1:C:215:CYS:HB2	1:C:248:LEU:HD12	1.96	0.47
1:A:67:GLY:HA3	1:A:278:TRP:CZ2	2.50	0.46
1:C:278:TRP:HE1	1:C:313:ASN:ND2	2.13	0.46
1:A:254:VAL:H	2:G:676:GLN:N	2.12	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:HD13	2:F:643:TYR:CE2	2.49	0.46
1:B:304:ILE:HD12	1:B:335:ASN:HB3	1.98	0.46
2:F:618:CYS:HB3	2:F:655:LYS:HD2	1.97	0.46
2:G:688:GLU:HA	2:G:691:ARG:HD2	1.95	0.46
1:C:229:SER:O	1:C:270:ILE:HD12	2.15	0.46
1:A:218:GLU:HA	1:A:223:PHE:HB3	1.98	0.46
2:G:556:GLU:H	2:G:556:GLU:CD	2.24	0.46
1:D:83:ARG:O	1:D:87:LYS:HB2	2.17	0.46
1:A:297:LYS:HG3	1:A:376:PRO:HG3	1.97	0.45
2:G:693:LEU:HG	2:G:694:PRO:HD2	1.98	0.45
1:A:302:GLU:O	1:A:305:PRO:HD2	2.15	0.45
1:A:274:ALA:HB3	1:A:308:LYS:HG3	1.99	0.45
1:C:249:TRP:O	1:C:277:ILE:HA	2.17	0.45
1:D:63:GLY:HA3	1:D:92:THR:O	2.16	0.45
2:H:650:ILE:HG23	2:H:651:MET:HE2	1.99	0.44
1:A:300:SER:O	1:A:303:LEU:HB2	2.16	0.44
1:C:213:LEU:HD12	1:C:246:GLU:HB2	2.00	0.44
2:E:636:ILE:HD12	2:E:637:LEU:H	1.83	0.44
1:B:314:PRO:HB2	1:B:321:ASN:OD1	2.17	0.44
2:H:604:ILE:O	2:H:608:ARG:HB2	2.18	0.44
1:D:81:LEU:HB2	1:D:318:PHE:HE1	1.82	0.43
1:D:225:TYR:O	1:D:232:PRO:HD2	2.18	0.43
1:A:214:PHE:HD2	1:A:247:VAL:HG13	1.84	0.43
2:E:579:LEU:HD21	2:H:688:GLU:HB3	2.00	0.43
1:B:172:LEU:HA	1:B:215:CYS:HB3	2.01	0.43
1:A:139:PRO:HG3	1:A:154:LEU:HD11	1.99	0.43
1:D:67:GLY:HA2	1:D:96:ALA:O	2.17	0.43
1:A:78:ARG:CB	1:A:122:LEU:HD11	2.48	0.43
1:C:329:ALA:C	1:C:333:LYS:HE2	2.44	0.43
1:A:107:TRP:HB2	1:A:137:ILE:HD11	2.00	0.42
1:C:261:VAL:HG22	1:C:303:LEU:HD13	2.01	0.42
2:E:560:LEU:HD23	2:E:624:MET:HG3	2.00	0.42
1:B:107:TRP:CZ2	1:B:143:ILE:HD12	2.54	0.42
2:H:679:TRP:C	2:H:681:PHE:H	2.27	0.42
1:B:63:GLY:HA3	1:B:92:THR:O	2.18	0.42
1:C:100:ASP:HB3	1:C:103:HIS:HB3	2.02	0.42
1:C:192:ALA:HB1	1:C:236:THR:HB	2.01	0.42
2:G:682:ARG:H	2:G:682:ARG:HG3	1.67	0.42
1:A:215:CYS:SG	3:A:501:OQ1:C12	3.08	0.42
1:A:67:GLY:HA2	1:A:96:ALA:O	2.20	0.42
2:G:560:LEU:HD11	2:G:621:VAL:HG22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:LEU:HD23	1:D:215:CYS:HB3	2.00	0.41
2:F:650:ILE:O	2:F:654:VAL:HG23	2.19	0.41
2:F:686:ALA:HB1	2:G:650:ILE:HD13	2.01	0.41
1:C:104:ARG:HB3	1:C:105:MET:H	1.72	0.41
2:G:560:LEU:O	2:G:564:LEU:HG	2.21	0.41
1:C:71:ARG:HA	1:C:72:PRO:HD3	1.90	0.41
1:D:120:MET:HE3	1:D:164:PHE:HA	2.02	0.41
1:C:70:GLY:H	1:C:99:ASP:CG	2.28	0.41
1:D:261:VAL:HA	1:D:264:ILE:HD12	2.01	0.41
1:D:286:TYR:CD1	2:H:679:TRP:HB3	2.55	0.41
2:H:683:GLY:HA3	2:H:687:GLY:HA3	2.01	0.41
1:B:268:SER:HA	1:B:273:ARG:O	2.21	0.41
2:F:625:PHE:CZ	2:F:647:ILE:HG23	2.55	0.41
1:D:134:ILE:HG21	1:D:213:LEU:HD13	2.02	0.41
1:A:69:TYR:CZ	1:A:98:LYS:HD2	2.56	0.41
1:B:74:VAL:HG22	1:B:77:GLN:OE1	2.21	0.41
2:H:656:SER:C	2:H:658:VAL:H	2.27	0.41
1:D:234:LEU:HA	1:D:237:VAL:HB	2.03	0.41
1:A:235:ARG:O	1:A:239:GLU:HB2	2.21	0.41
1:C:221:GLY:HA2	1:C:228:VAL:CG2	2.51	0.41
1:C:67:GLY:HA2	1:C:96:ALA:O	2.21	0.41
1:C:88:TRP:HZ2	1:C:322:TYR:CZ	2.39	0.41
1:A:101:TYR:N	1:A:101:TYR:CD1	2.89	0.40
1:C:333:LYS:HA	1:C:336:MET:HE2	2.03	0.40
1:D:97:PRO:HB2	1:D:100:ASP:HB2	2.03	0.40
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.99	0.40
1:A:270:ILE:H	1:A:270:ILE:HG13	1.71	0.40
1:D:103:HIS:HD2	1:D:137:ILE:HA	1.85	0.40
1:A:96:ALA:N	1:A:97:PRO:HD3	2.36	0.40
1:C:275:PRO:HD2	1:C:307:LEU:HD23	2.02	0.40
1:D:71:ARG:NE	2:H:641:TYR:CD2	2.79	0.40
1:D:215:CYS:SG	3:D:501:OQ1:C12	3.09	0.40
1:A:171:LEU:HD12	1:A:199:THR:HA	2.03	0.40
1:D:275:PRO:HD2	1:D:307:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/388 (79%)	287 (94%)	17 (6%)	1 (0%)	36	54
1	B	305/388 (79%)	286 (94%)	16 (5%)	3 (1%)	12	25
1	C	304/388 (78%)	275 (90%)	24 (8%)	5 (2%)	7	17
1	D	304/388 (78%)	279 (92%)	21 (7%)	4 (1%)	9	21
2	E	106/161 (66%)	97 (92%)	6 (6%)	3 (3%)	4	9
2	F	103/161 (64%)	98 (95%)	5 (5%)	0	100	100
2	G	111/161 (69%)	105 (95%)	4 (4%)	2 (2%)	6	15
2	H	106/161 (66%)	99 (93%)	6 (6%)	1 (1%)	14	28
All	All	1644/2196 (75%)	1526 (93%)	99 (6%)	19 (1%)	10	22

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	677	GLU
2	G	680	ALA
1	C	57	ALA
1	D	140	GLY
1	D	181	CYS
1	C	140	GLY
1	C	141	LEU
2	E	566	TYR
2	H	681	PHE
1	B	105	MET
1	B	182	ALA
1	C	58	ARG
2	E	678	PRO
2	E	680	ALA
1	A	314	PRO
1	C	105	MET
1	D	57	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	314	PRO
1	B	314	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/331 (84%)	255 (92%)	22 (8%)	11	24
1	B	276/331 (83%)	254 (92%)	22 (8%)	11	24
1	C	270/331 (82%)	243 (90%)	27 (10%)	7	16
1	D	270/331 (82%)	244 (90%)	26 (10%)	8	17
2	E	95/140 (68%)	79 (83%)	16 (17%)	2	3
2	F	94/140 (67%)	84 (89%)	10 (11%)	6	13
2	G	102/140 (73%)	90 (88%)	12 (12%)	5	10
2	H	96/140 (69%)	82 (85%)	14 (15%)	3	5
All	All	1480/1884 (79%)	1331 (90%)	149 (10%)	7	15

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	76	GLU
1	A	100	ASP
1	A	114	GLU
1	A	118	GLN
1	A	121	THR
1	A	144	THR
1	A	154	LEU
1	A	157	LYS
1	A	228	VAL
1	A	229	SER
1	A	247	VAL
1	A	257	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	258	GLU
1	A	264	ILE
1	A	265	GLU
1	A	270	ILE
1	A	278	TRP
1	A	301	THR
1	A	317	GLU
1	A	337	ASN
1	A	378	MET
1	B	64	VAL
1	B	65	VAL
1	B	128	GLU
1	B	132	GLU
1	B	143	ILE
1	B	144	THR
1	B	167	ARG
1	B	177	ASP
1	B	185	LYS
1	B	206	LEU
1	B	210	GLU
1	B	240	LYS
1	B	241	LEU
1	B	246	GLU
1	B	257	LYS
1	B	262	GLU
1	B	267	VAL
1	B	279	ASP
1	B	290	ARG
1	B	317	GLU
1	B	336	MET
1	B	372	VAL
1	C	59	ARG
1	C	61	LEU
1	C	83	ARG
1	C	89	GLU
1	C	114	GLU
1	C	118	GLN
1	C	124	SER
1	C	130	GLU
1	C	137	ILE
1	C	138	SER
1	C	151	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	171	LEU
1	C	229	SER
1	C	246	GLU
1	C	253	LYS
1	C	258	GLU
1	C	262	GLU
1	C	264	ILE
1	C	281	ILE
1	C	288	GLN
1	C	289	LYS
1	C	302	GLU
1	C	303	LEU
1	C	317	GLU
1	C	340	ARG
1	C	370	THR
1	C	385	THR
1	D	50	VAL
1	D	59	ARG
1	D	71	ARG
1	D	83	ARG
1	D	87	LYS
1	D	98	LYS
1	D	102	LYS
1	D	103	HIS
1	D	120	MET
1	D	142	ASP
1	D	143	ILE
1	D	149	LYS
1	D	153	THR
1	D	189	SER
1	D	227	ASN
1	D	246	GLU
1	D	257	LYS
1	D	258	GLU
1	D	278	TRP
1	D	281	ILE
1	D	317	GLU
1	D	334	SER
1	D	339	VAL
1	D	378	MET
1	D	382	LEU
1	D	390	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	574	LYS
2	E	577	GLN
2	E	602	GLU
2	E	608	ARG
2	E	620	LEU
2	E	628	LEU
2	E	629	SER
2	E	636	ILE
2	E	640	MET
2	E	647	ILE
2	E	654	VAL
2	E	677	GLU
2	E	679	TRP
2	E	682	ARG
2	E	685	LEU
2	E	693	LEU
2	F	554	THR
2	F	583	GLN
2	F	604	ILE
2	F	618	CYS
2	F	631	CYS
2	F	639	ASP
2	F	650	ILE
2	F	656	SER
2	F	659	GLN
2	F	691	ARG
2	G	588	ASN
2	G	600	ASP
2	G	606	GLU
2	G	613	LYS
2	G	620	LEU
2	G	639	ASP
2	G	640	MET
2	G	647	ILE
2	G	650	ILE
2	G	656	SER
2	G	688	GLU
2	G	693	LEU
2	H	570	GLU
2	H	579	LEU
2	H	608	ARG
2	H	618	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	620	LEU
2	H	626	THR
2	H	628	LEU
2	H	639	ASP
2	H	644	VAL
2	H	646	ASP
2	H	650	ILE
2	H	676	GLN
2	H	681	PHE
2	H	685	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	230	GLN
1	A	284	ASN
1	A	335	ASN
1	C	118	GLN
1	C	195	GLN
1	C	389	GLN
1	D	86	GLN
1	D	204	GLN
1	D	227	ASN
2	E	583	GLN
2	E	630	ASN
2	E	690	GLN
2	F	583	GLN
2	G	583	GLN
2	G	588	ASN
2	G	690	GLN
2	H	559	GLN
2	H	583	GLN
2	H	630	ASN

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OQ1	D	501	-	16,18,18	0.69	0	14,26,26	1.58	3 (21%)
3	OQ1	A	501	-	16,18,18	0.63	0	14,26,26	1.53	3 (21%)
3	OQ1	B	501	-	16,18,18	0.68	0	14,26,26	0.87	0
3	OQ1	C	501	-	16,18,18	0.79	1 (6%)	14,26,26	2.79	7 (50%)

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	OQ1	D	501	-	-	4/7/35/35	0/2/2/2
3	OQ1	A	501	-	-	4/7/35/35	0/2/2/2
3	OQ1	B	501	-	-	1/7/35/35	0/2/2/2
3	OQ1	C	501	-	-	3/7/35/35	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	OQ1	C2-C3	-2.02	1.50	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	OQ1	C4-O-C	6.40	122.56	114.17
3	C	501	OQ1	O-C-C1	4.87	114.82	107.94
3	D	501	OQ1	C4-O-C	3.92	119.32	114.17
3	A	501	OQ1	F1-C5-F	3.83	112.92	105.53
3	C	501	OQ1	C2-C3-N	-3.28	105.97	110.56
3	C	501	OQ1	O-C4-C3	2.70	121.20	115.27
3	A	501	OQ1	C2-C3-N	-2.56	106.97	110.56
3	C	501	OQ1	F1-C5-F	-2.56	100.59	105.53
3	C	501	OQ1	O7-C1-C2	-2.46	104.59	110.38
3	C	501	OQ1	N10-C9-N	2.44	127.39	124.28
3	A	501	OQ1	C5-C-C1	2.27	117.79	113.42
3	D	501	OQ1	C2-C3-N	-2.20	107.48	110.56
3	D	501	OQ1	O-C4-C3	2.12	119.94	115.27

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	OQ1	C1-C-C5-F
3	A	501	OQ1	O-C-C5-F
3	A	501	OQ1	C1-C-C5-F1
3	A	501	OQ1	O-C-C5-F1
3	B	501	OQ1	O-C-C5-F1
3	C	501	OQ1	O-C-C5-F
3	C	501	OQ1	C1-C-C5-F1
3	C	501	OQ1	O-C-C5-F1
3	D	501	OQ1	C1-C-C5-F
3	D	501	OQ1	O-C-C5-F
3	D	501	OQ1	C1-C-C5-F1
3	D	501	OQ1	O-C-C5-F1

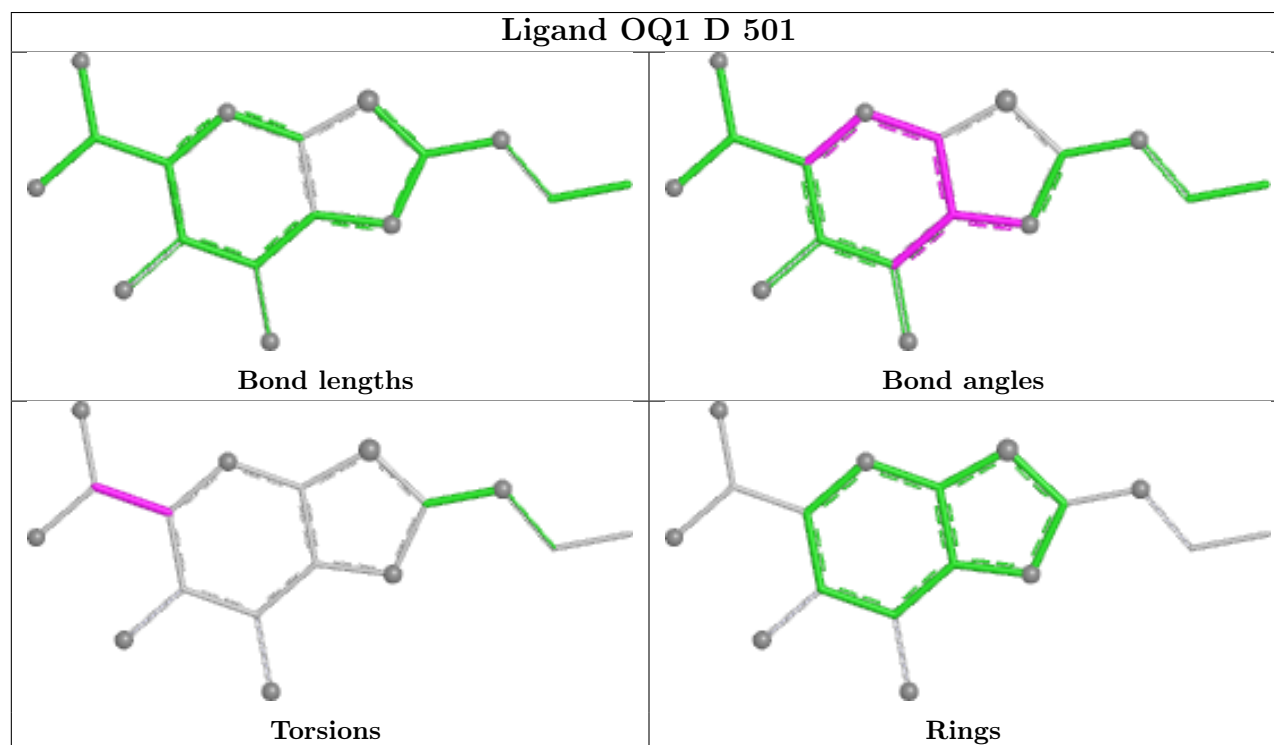
There are no ring outliers.

2 monomers are involved in 2 short contacts:

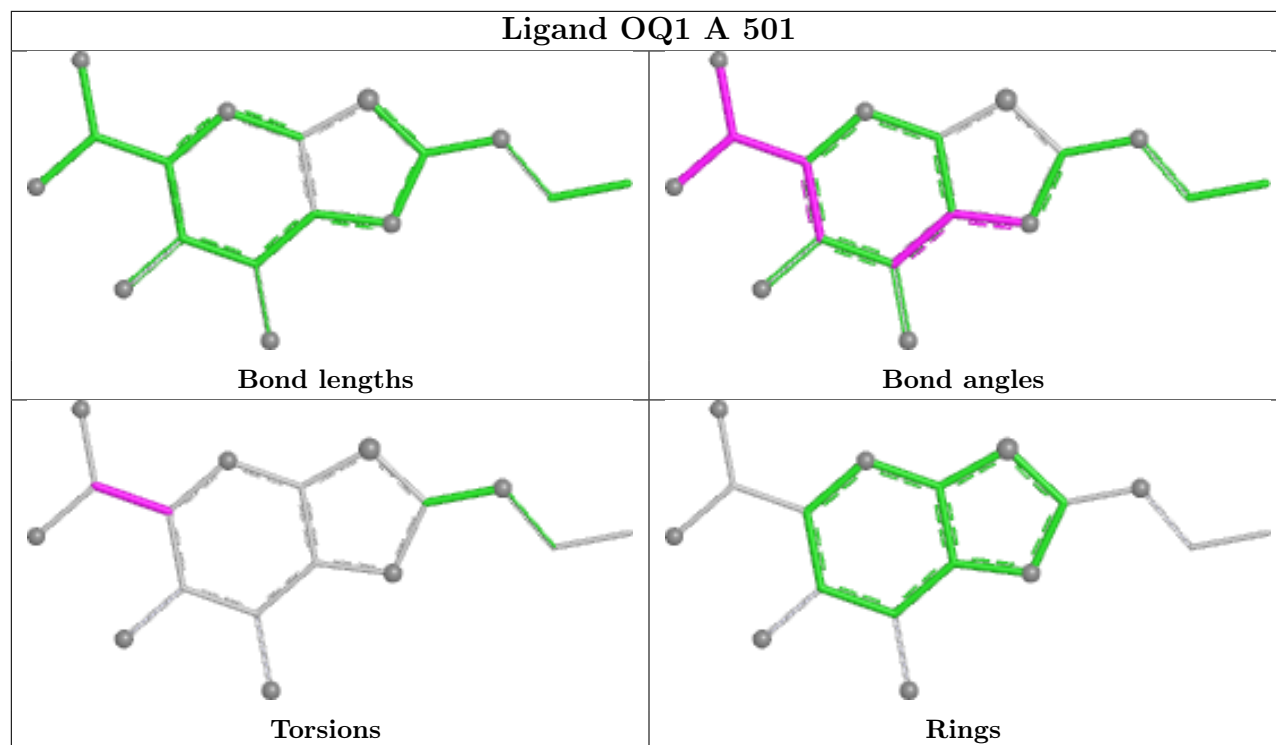
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	OQ1	1	0
3	A	501	OQ1	1	0

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

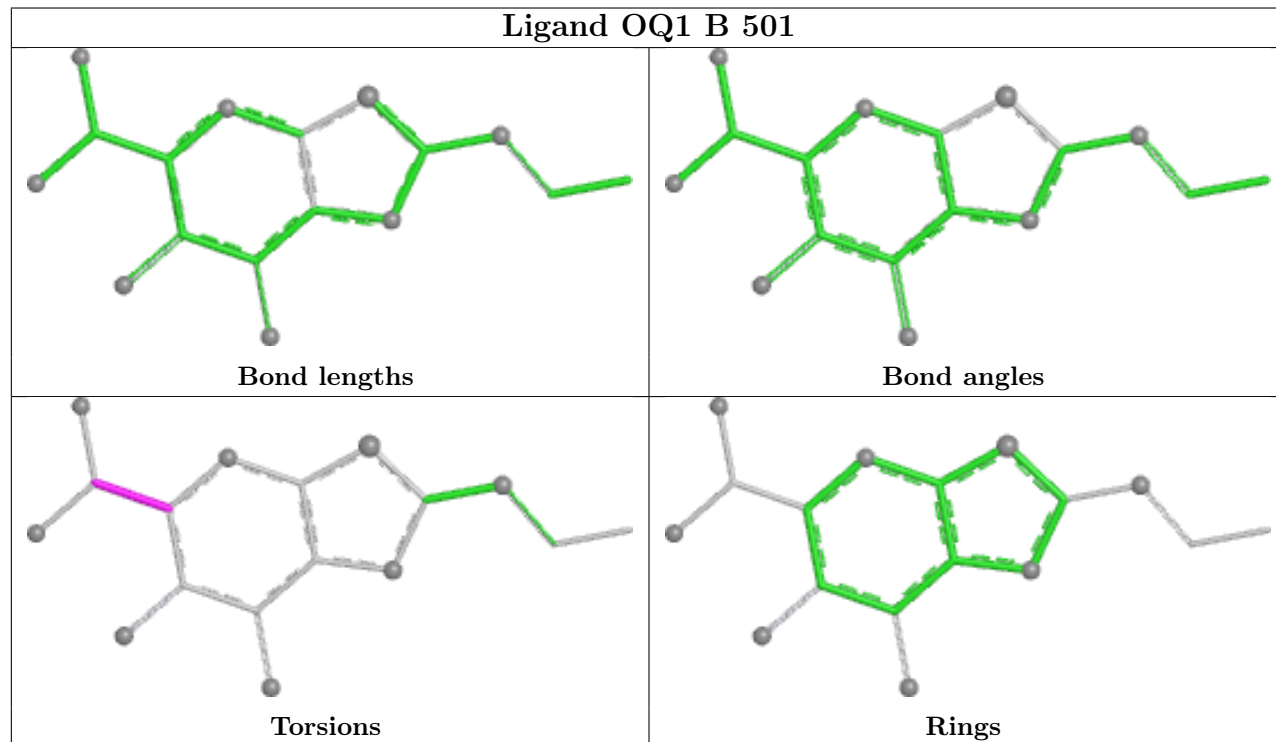
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

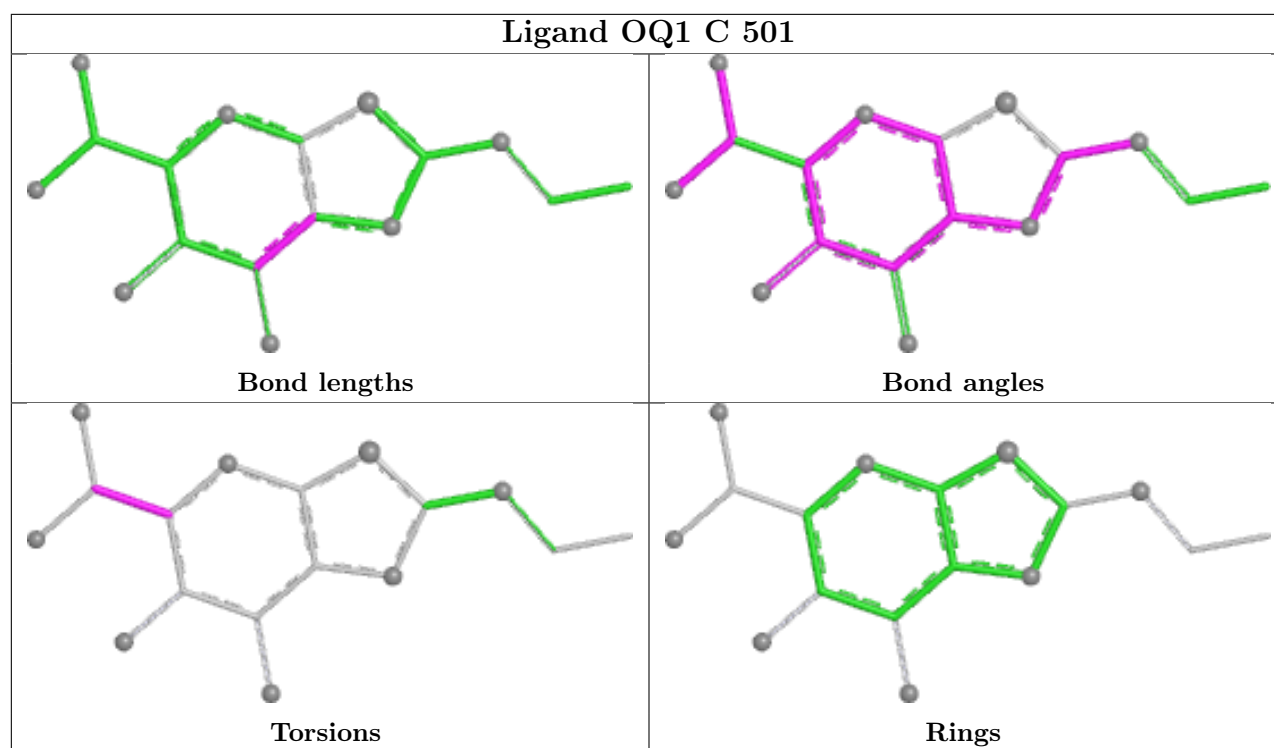


Ligand OQ1 A 501



Ligand OQ1 B 501





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	309/388 (79%)	0.17	4 (1%) 75 68	35, 51, 70, 88	0
1	B	309/388 (79%)	-0.05	3 (0%) 79 74	33, 47, 63, 76	0
1	C	310/388 (79%)	0.28	9 (2%) 53 45	35, 53, 75, 99	0
1	D	310/388 (79%)	0.57	8 (2%) 57 48	37, 67, 96, 116	0
2	E	112/161 (69%)	1.10	18 (16%) 4 4	55, 84, 117, 129	0
2	F	109/161 (67%)	0.72	11 (10%) 12 10	41, 60, 82, 96	0
2	G	117/161 (72%)	0.70	9 (7%) 19 14	34, 59, 88, 106	0
2	H	112/161 (69%)	1.23	22 (19%) 3 3	47, 78, 113, 134	0
All	All	1688/2196 (76%)	0.43	84 (4%) 34 27	33, 56, 95, 134	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	601	SER	5.3
2	G	680	ALA	4.3
2	E	645	TRP	4.0
2	E	677	GLU	3.8
2	H	641	TYR	3.7
2	H	649	SER	3.6
1	C	49	ALA	3.5
2	H	586	ARG	3.4
2	H	604	ILE	3.1
2	G	677	GLU	3.1
2	H	625	PHE	3.0
2	E	692	LEU	3.0
1	A	225	TYR	2.9
2	E	554	THR	2.9
2	H	645	TRP	2.8
2	H	575	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	57	ALA	2.7
1	C	96	ALA	2.7
1	D	148	PRO	2.6
2	G	599	LYS	2.6
2	H	658	VAL	2.6
2	F	612	ALA	2.6
2	E	633	ASN	2.5
2	F	589	SER	2.5
2	F	604	ILE	2.5
2	H	631	CYS	2.5
1	A	372	VAL	2.5
2	H	657	PHE	2.5
2	E	604	ILE	2.4
2	G	695	ILE	2.4
2	E	601	SER	2.4
2	E	632	ALA	2.4
2	H	628	LEU	2.4
1	C	267	VAL	2.4
2	H	677	GLU	2.4
1	D	101	TYR	2.4
2	F	564	LEU	2.4
1	D	139	PRO	2.4
2	H	557	ASP	2.4
2	E	655	LYS	2.4
2	H	685	LEU	2.4
2	E	678	PRO	2.4
2	F	617	MET	2.3
2	E	602	GLU	2.3
2	E	605	GLU	2.3
2	G	617	MET	2.3
2	H	637	LEU	2.3
1	D	145	PHE	2.3
2	F	695	ILE	2.3
2	G	656	SER	2.3
1	D	106	PHE	2.3
2	F	603	LYS	2.3
1	B	278	TRP	2.3
2	G	681	PHE	2.2
1	B	397	TYR	2.2
2	F	608	ARG	2.2
1	D	153	THR	2.2
1	A	275	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	50	VAL	2.2
2	F	683	GLY	2.2
2	H	555	LEU	2.2
2	G	676	GLN	2.2
1	A	178	HIS	2.2
2	E	585	LEU	2.2
1	C	182	ALA	2.2
1	D	140	GLY	2.1
1	C	101	TYR	2.1
2	H	642	SER	2.1
1	C	99	ASP	2.1
2	E	626	THR	2.1
2	F	620	LEU	2.1
2	H	601	SER	2.1
1	B	289	LYS	2.1
2	E	685	LEU	2.1
1	D	57	ALA	2.1
2	H	638	TYR	2.1
2	E	625	PHE	2.0
2	E	629	SER	2.0
2	E	652	SER	2.0
2	F	582	PHE	2.0
2	H	611	ALA	2.0
1	C	100	ASP	2.0
2	H	622	MET	2.0
2	H	660	TRP	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](#)

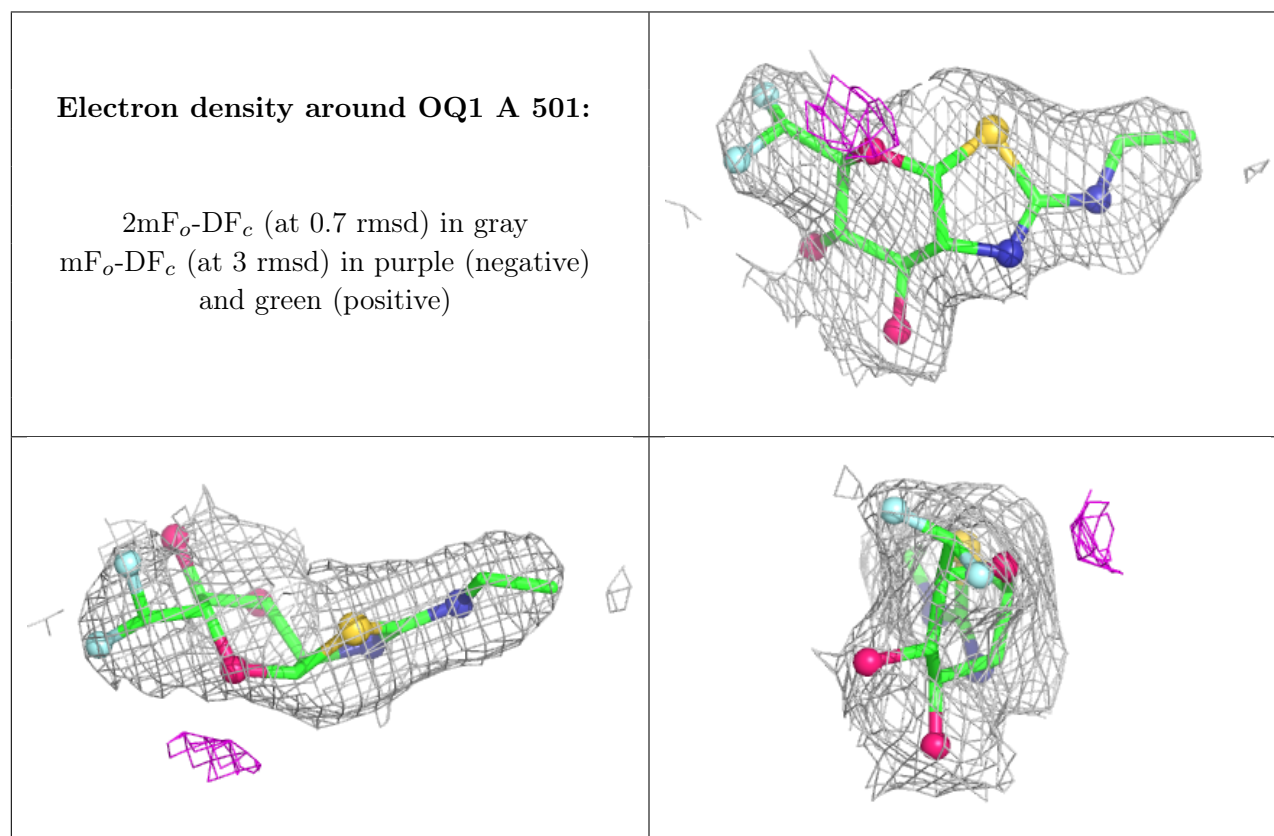
There are no oligosaccharides in this entry.

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.

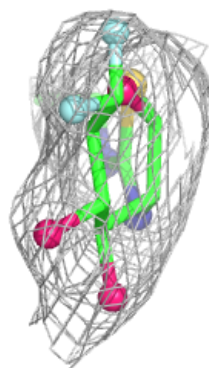
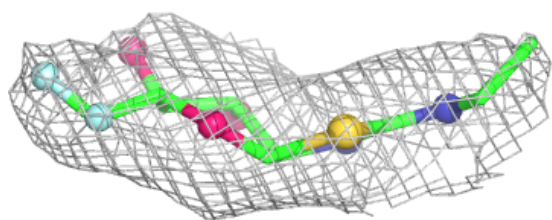
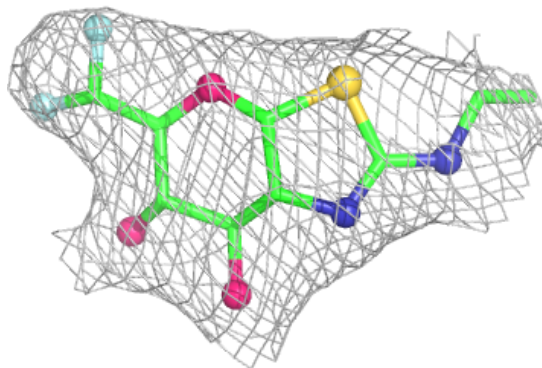
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OQ1	A	501	17/17	0.91	0.11	29,54,59,59	0
3	OQ1	C	501	17/17	0.93	0.10	44,52,57,57	0
3	OQ1	D	501	17/17	0.94	0.12	49,52,58,58	0
3	OQ1	B	501	17/17	0.95	0.10	25,45,55,57	0

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.

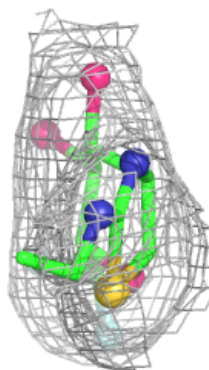
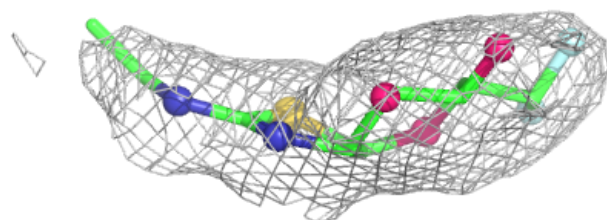
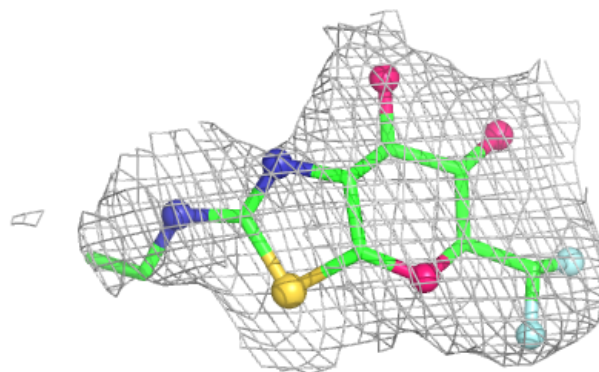


Electron density around OQ1 C 501:

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

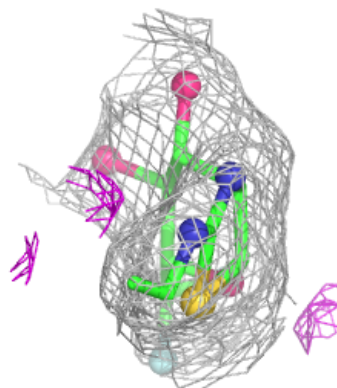
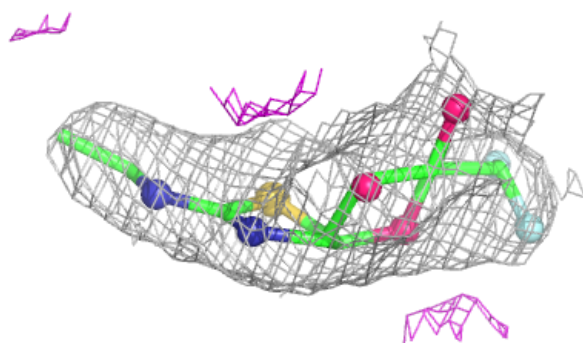
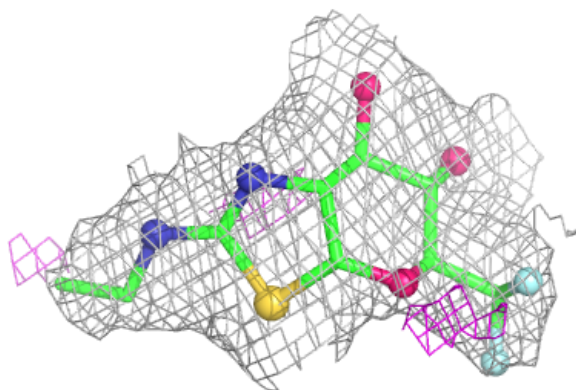
**Electron density around OQ1 D 501:**

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



Electron density around OQ1 B 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.