



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:37 PM UTC

PDB ID : 3KWF / pdb_00003kwf
Title : human DPP-IV with carmegliptin (S)-1-((2S,3S,11bS)-2-Amino-9,10-dimethoxy-1,3,4,6,7,11b-hexahydro-2H-pyrido[2,1-a]isoquinolin-3-yl)-4-fluoromethyl-pyrrolidin-2-one
Authors : Hennig, M.; Stihle, M.; Thoma, R.
Deposited on : 2009-12-01
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

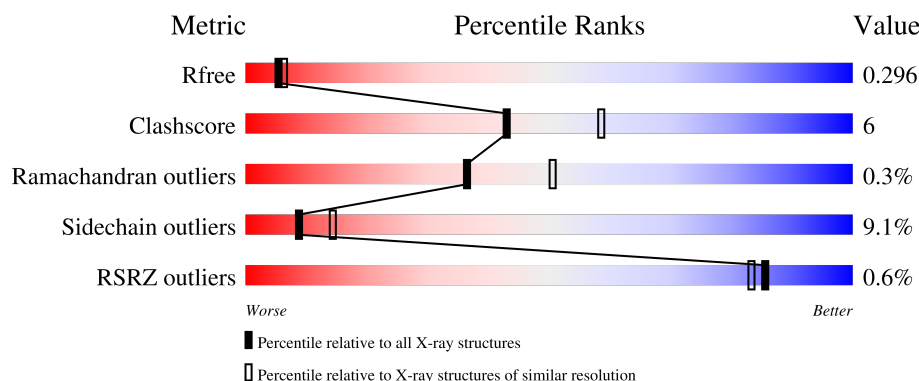
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	728	83% 14% .
1	B	728	81% 16% .

2 Entry composition [i](#)

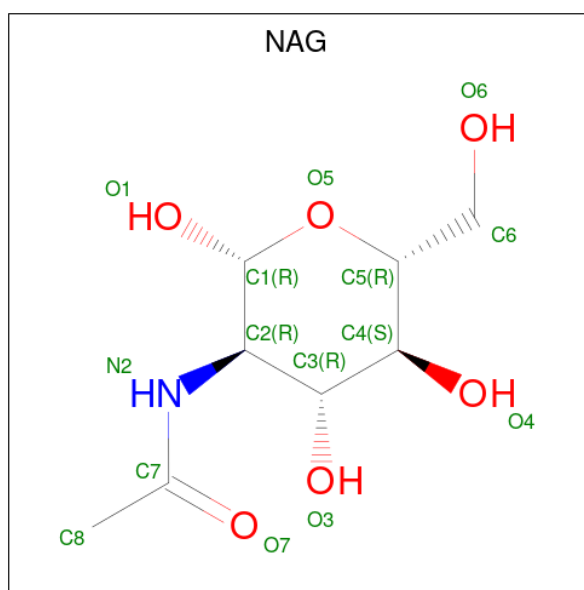
There are 4 unique types of molecules in this entry. The entry contains 12464 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

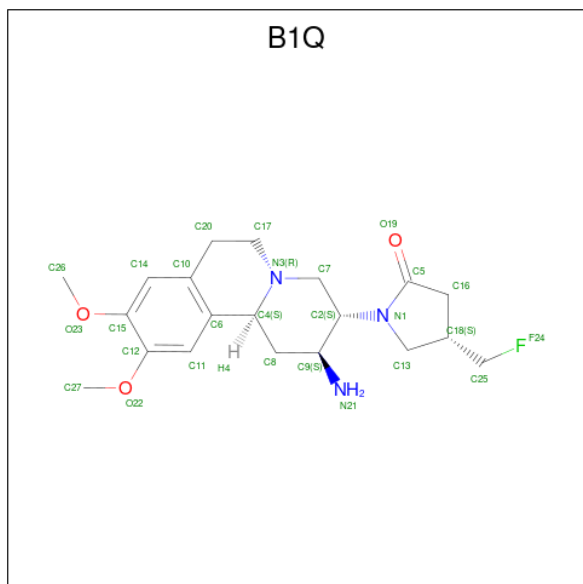
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (4S)-1-[(2S,3S,11bS)-2-amino-9,10-dimethoxy-1,3,4,6,7,11b-hexahydro-2H-pyrido[2,1-a]isoquinolin-3-yl]-4-(fluoromethyl)pyrrolidin-2-one (CCD ID: B1Q) (formula: $C_{20}H_{28}FN_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			27	20	1	3	3		
3	B	1	Total	C	F	N	O	0	0
			27	20	1	3	3		

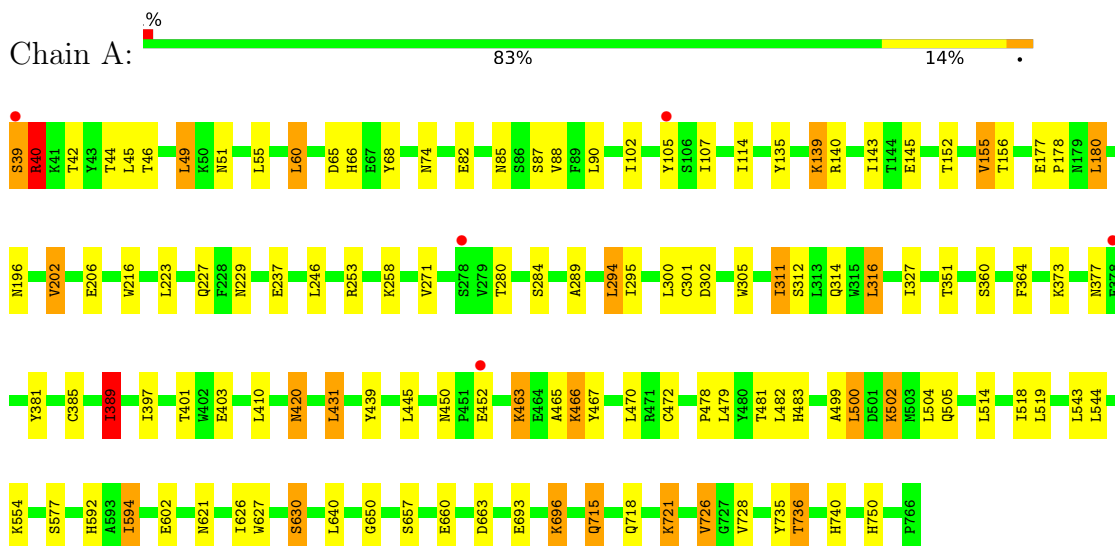
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total	O	0	0
			203	203		
4	B	225	Total	O	0	0
			225	225		

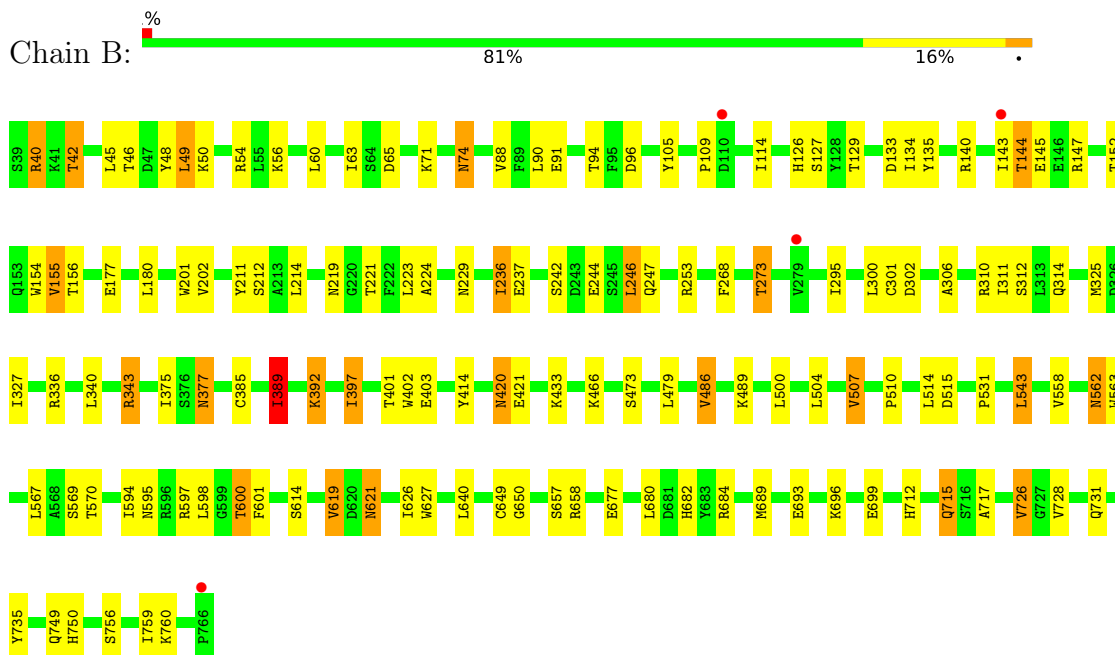
3 Residue-property plots [i](#)

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: Dipeptidyl peptidase 4



- Molecule 1: Dipeptidyl peptidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.63Å 69.54Å 423.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	88.0 (15.00-2.40) 87.5 (15.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.246 (Not available) , 0.296	Depositor DCC
R_{free} test set	3425 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12464	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: NAG, B1Q

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	0.59	0/6135	0.83	3/8344 (0.0%)
1	B	0.60	1/6135 (0.0%)	0.86	5/8344 (0.1%)
All	All	0.60	1/12270 (0.0%)	0.84	8/16688 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	531	PRO	CA-C	5.04	1.54	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ILE	N-CA-C	9.02	119.83	110.72
1	B	389	ILE	N-CA-C	8.79	119.58	110.62
1	A	202	VAL	N-CA-C	6.26	117.05	110.72
1	B	392	LYS	N-CA-C	6.26	117.90	111.14
1	B	397	ILE	N-CA-C	-5.63	108.02	113.53
1	B	96	ASP	N-CA-C	-5.32	106.92	113.41
1	B	201	TRP	N-CA-C	5.23	117.39	111.11
1	A	40	ARG	N-CA-C	5.14	121.75	110.80

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	5963	0	5685	75	0
1	B	5963	0	5684	78	0
2	A	28	0	26	6	0
2	B	28	0	26	2	0
3	A	27	0	28	0	0
3	B	27	0	28	0	0
4	A	203	0	0	10	0
4	B	225	0	0	13	0
All	All	12464	0	11477	146	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 (146) 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:85:ASN:HD21	2:A:794:NAG:C1	1.24	1.49
1:B:229:ASN:HD21	2:B:796:NAG:C1	1.30	1.45
1:A:85:ASN:ND2	2:A:794:NAG:C1	1.93	1.29
1:A:229:ASN:HD21	2:A:796:NAG:C1	1.48	1.24
1:B:229:ASN:ND2	2:B:796:NAG:C1	2.15	1.10
1:B:600:THR:CG2	1:B:601:PHE:H	1.66	1.09
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.46	0.97
1:B:600:THR:HG23	1:B:601:PHE:H	1.29	0.96
1:A:229:ASN:ND2	2:A:796:NAG:C1	2.28	0.95
1:B:65:ASP:HB2	4:B:975:HOH:O	1.69	0.92
1:A:630:SER:HB3	1:A:740:HIS:NE2	1.87	0.90
1:B:600:THR:HG23	1:B:601:PHE:N	1.87	0.85
1:A:466:LYS:HG2	4:A:944:HOH:O	1.79	0.81
1:B:600:THR:HG22	1:B:601:PHE:H	1.50	0.77
1:B:56:LYS:HE3	4:B:767:HOH:O	1.83	0.77
1:B:403:GLU:H	1:B:420:ASN:HD21	1.32	0.77
1:A:630:SER:HB3	1:A:740:HIS:CE1	2.22	0.74
1:A:431:LEU:HD13	1:A:445:LEU:HD12	1.69	0.72
1:A:44:THR:HG22	1:A:46:THR:H	1.55	0.72
1:B:726:VAL:HG12	1:B:728:VAL:HG23	1.73	0.70
1:A:736:THR:HG21	1:B:717:ALA:O	1.93	0.68
1:A:39:SER:N	4:A:871:HOH:O	2.26	0.67
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.77	0.67
1:A:403:GLU:H	1:A:420:ASN:HD21	1.42	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:LYS:HB2	4:B:975:HOH:O	1.96	0.66
1:B:735:TYR:OH	1:B:750:HIS:HD2	1.79	0.64
1:A:693:GLU:O	1:A:696:LYS:HG3	1.97	0.64
1:A:450:ASN:OD1	4:A:25:HOH:O	2.14	0.63
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.79	0.63
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.80	0.63
1:B:657:SER:H	1:B:715:GLN:NE2	1.97	0.63
1:B:54:ARG:HD2	4:B:767:HOH:O	1.98	0.63
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.79	0.62
1:B:600:THR:CG2	1:B:601:PHE:N	2.35	0.62
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.83	0.61
1:B:126:HIS:HD2	4:B:24:HOH:O	1.83	0.61
1:A:44:THR:HG22	1:A:46:THR:N	2.16	0.60
1:B:327:ILE:HD13	1:B:389:ILE:HG12	1.84	0.60
1:B:598:LEU:O	1:B:682:HIS:HE1	1.85	0.59
1:B:658:ARG:HB2	1:B:689:MET:HE1	1.85	0.59
1:A:85:ASN:ND2	2:A:794:NAG:O5	2.35	0.59
1:B:42:THR:HG23	1:B:570:THR:OG1	2.03	0.59
1:B:312:SER:OG	1:B:325:MET:HE3	2.03	0.58
1:B:562:ASN:C	1:B:562:ASN:HD22	2.11	0.57
1:B:42:THR:HG22	4:B:780:HOH:O	2.03	0.57
1:B:134:ILE:HB	1:B:143:ILE:HG12	1.85	0.57
1:B:377:ASN:C	1:B:377:ASN:HD22	2.11	0.56
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.85	0.56
1:A:657:SER:H	1:A:715:GLN:NE2	2.03	0.56
1:B:145:GLU:HG3	4:B:858:HOH:O	2.05	0.56
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.41	0.56
1:A:718:GLN:OE1	1:A:721:LYS:NZ	2.39	0.56
1:A:253:ARG:HH12	1:B:253:ARG:NH1	2.04	0.55
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.89	0.55
1:B:403:GLU:H	1:B:420:ASN:ND2	2.03	0.54
1:A:253:ARG:NH1	1:B:253:ARG:HH12	2.06	0.53
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.91	0.53
1:B:340:LEU:HB2	1:B:343:ARG:HD2	1.90	0.53
1:A:295:ILE:HG23	4:A:834:HOH:O	2.07	0.53
1:A:499:ALA:O	1:A:502:LYS:HG3	2.08	0.53
1:A:377:ASN:HD22	1:A:377:ASN:C	2.16	0.52
1:A:65:ASP:HB2	4:A:944:HOH:O	2.10	0.52
1:A:229:ASN:ND2	2:A:796:NAG:O5	2.37	0.52
1:B:486:VAL:HG23	4:B:911:HOH:O	2.09	0.52
1:A:750:HIS:HE1	1:B:728:VAL:O	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.91	0.51
1:A:305:TRP:CZ3	1:A:311:ILE:HG12	2.45	0.51
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.92	0.51
1:A:139:LYS:O	1:A:140:ARG:HG3	2.11	0.50
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.94	0.50
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.11	0.50
1:A:327:ILE:HD13	1:A:389:ILE:HG12	1.93	0.50
1:A:401:THR:HG22	1:A:401:THR:O	2.12	0.50
1:A:500:LEU:HD22	1:A:504:LEU:HG	1.94	0.50
1:B:563:TRP:CH2	1:B:759:ILE:HD12	2.47	0.50
1:A:289:ALA:HB3	1:A:294:LEU:HD13	1.93	0.50
1:A:420:ASN:C	1:A:420:ASN:HD22	2.21	0.49
1:A:44:THR:CG2	4:A:942:HOH:O	2.61	0.49
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.95	0.49
1:A:502:LYS:HD3	4:A:900:HOH:O	2.13	0.48
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.96	0.48
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.49	0.48
1:B:614:SER:HA	1:B:619:VAL:CG2	2.43	0.47
1:B:598:LEU:O	1:B:682:HIS:CE1	2.67	0.47
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.50	0.47
1:B:401:THR:HG22	1:B:401:THR:O	2.12	0.47
1:B:414:TYR:CE1	1:B:433:LYS:HE2	2.50	0.47
1:A:463:LYS:C	1:A:465:ALA:H	2.23	0.47
1:A:82:GLU:HB2	1:A:467:TYR:OH	2.15	0.46
1:A:66:HIS:HB2	4:A:828:HOH:O	2.13	0.46
1:B:133:ASP:OD1	1:B:147:ARG:NH1	2.48	0.46
1:B:657:SER:H	1:B:715:GLN:HE21	1.63	0.46
1:A:626:ILE:O	1:A:650:GLY:HA2	2.16	0.46
1:A:377:ASN:ND2	1:A:381:TYR:H	2.14	0.46
1:B:504:LEU:HA	1:B:507:VAL:HG13	1.98	0.45
1:A:45:LEU:HG	1:A:49:LEU:HD22	1.99	0.45
1:B:221:THR:O	1:B:273:THR:HB	2.17	0.45
1:B:543:LEU:HD12	1:B:567:LEU:HD13	1.99	0.45
1:A:519:LEU:HD23	1:A:519:LEU:HA	1.75	0.45
1:B:756:SER:O	1:B:760:LYS:HG3	2.16	0.45
1:A:44:THR:HG23	4:A:942:HOH:O	2.17	0.44
1:A:728:VAL:O	1:B:750:HIS:HE1	2.01	0.44
1:B:595:ASN:O	1:B:597:ARG:NE	2.49	0.44
1:B:649:CYS:HB3	1:B:699:GLU:HB2	2.00	0.44
1:A:55:LEU:HD22	1:A:478:PRO:HG2	2.00	0.44
1:A:351:THR:OG1	1:A:592:HIS:HD2	2.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLU:H	1:A:420:ASN:ND2	2.11	0.44
1:A:143:ILE:HD13	1:A:178:PRO:HB2	2.00	0.44
1:A:60:LEU:HB2	1:A:68:TYR:CD1	2.53	0.43
1:B:242:SER:HB3	1:B:246:LEU:HD12	2.00	0.43
1:A:657:SER:H	1:A:715:GLN:HE21	1.66	0.43
1:B:144:THR:HB	4:B:858:HOH:O	2.17	0.43
1:B:377:ASN:C	1:B:377:ASN:ND2	2.76	0.43
1:A:364:PHE:HE1	1:A:389:ILE:HD11	1.84	0.43
1:B:236:ILE:HG13	1:B:712:HIS:CE1	2.54	0.43
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.35	0.43
1:A:594:ILE:HD11	1:A:602:GLU:OE1	2.19	0.43
1:B:40:ARG:NH1	4:B:978:HOH:O	2.52	0.43
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.54	0.43
1:B:42:THR:CG2	1:B:570:THR:OG1	2.66	0.42
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.99	0.42
1:A:156:THR:HG23	1:A:216:TRP:HE1	1.84	0.42
1:B:49:LEU:HG	1:B:749:GLN:HG2	2.01	0.42
1:B:219:ASN:ND2	4:B:812:HOH:O	2.51	0.42
1:A:735:TYR:OH	1:A:750:HIS:HD2	2.01	0.42
1:A:253:ARG:HH12	1:B:253:ARG:HH12	1.60	0.42
1:A:554:LYS:HB3	1:A:577:SER:HB3	2.01	0.42
1:A:301:CYS:SG	1:A:316:LEU:HB2	2.60	0.41
1:A:152:THR:HG21	1:A:155:VAL:HG22	2.02	0.41
1:A:360:SER:O	1:A:373:LYS:NZ	2.48	0.41
1:B:152:THR:HG21	1:B:155:VAL:HG22	2.02	0.41
1:B:621:ASN:HD22	1:B:621:ASN:C	2.28	0.41
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.55	0.41
1:A:592:HIS:HE1	4:A:865:HOH:O	2.03	0.41
1:B:597:ARG:HA	1:B:682:HIS:CE1	2.55	0.41
1:B:127:SER:HB3	1:B:211:TYR:CD1	2.55	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.20	0.41
1:B:48:TYR:CE1	1:B:562:ASN:HA	2.56	0.41
1:B:420:ASN:C	1:B:420:ASN:HD22	2.28	0.41
1:A:258:LYS:HD2	1:B:247:GLN:HG2	2.03	0.41
1:A:271:VAL:HG22	1:A:284:SER:HA	2.02	0.41
1:A:302:ASP:HB3	1:A:314:GLN:HB2	2.03	0.41
1:A:381:TYR:CZ	1:A:401:THR:HG23	2.56	0.40
1:B:693:GLU:HG2	4:B:905:HOH:O	2.21	0.40
1:B:433:LYS:HE3	4:B:28:HOH:O	2.21	0.40
1:B:114:ILE:HG23	1:B:135:TYR:HB3	2.03	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	726/728 (100%)	689 (95%)	34 (5%)	3 (0%)	30	43
1	B	726/728 (100%)	688 (95%)	36 (5%)	2 (0%)	36	50
All	All	1452/1456 (100%)	1377 (95%)	70 (5%)	5 (0%)	36	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	74	ASN
1	A	139	LYS
1	A	40	ARG
1	A	630	SER
1	B	109	PRO

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	572/653 (88%)	521 (91%)	51 (9%)	9	15
1	B	653/653 (100%)	592 (91%)	61 (9%)	8	14
All	All	1225/1306 (94%)	1113 (91%)	112 (9%)	9	14

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	ARG
1	A	42	THR
1	A	49	LEU
1	A	51	ASN
1	A	60	LEU
1	A	74	ASN
1	A	87	SER
1	A	88	VAL
1	A	90	LEU
1	A	102	ILE
1	A	107	ILE
1	A	145	GLU
1	A	155	VAL
1	A	180	LEU
1	A	202	VAL
1	A	223	LEU
1	A	246	LEU
1	A	280	THR
1	A	294	LEU
1	A	300	LEU
1	A	311	ILE
1	A	312	SER
1	A	316	LEU
1	A	385	CYS
1	A	389	ILE
1	A	410	LEU
1	A	420	ASN
1	A	431	LEU
1	A	452	GLU
1	A	463	LYS
1	A	466	LYS
1	A	472	CYS
1	A	479	LEU
1	A	482	LEU
1	A	500	LEU
1	A	502	LYS
1	A	505	GLN
1	A	514	LEU
1	A	518	ILE
1	A	543	LEU
1	A	544	LEU
1	A	594	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	621	ASN
1	A	627	TRP
1	A	660	GLU
1	A	696	LYS
1	A	715	GLN
1	A	721	LYS
1	A	726	VAL
1	A	736	THR
1	B	40	ARG
1	B	42	THR
1	B	46	THR
1	B	49	LEU
1	B	50	LYS
1	B	60	LEU
1	B	63	ILE
1	B	71	LYS
1	B	74	ASN
1	B	88	VAL
1	B	90	LEU
1	B	91	GLU
1	B	94	THR
1	B	129	THR
1	B	140	ARG
1	B	144	THR
1	B	155	VAL
1	B	156	THR
1	B	202	VAL
1	B	214	LEU
1	B	223	LEU
1	B	236	ILE
1	B	244	GLU
1	B	246	LEU
1	B	273	THR
1	B	295	ILE
1	B	300	LEU
1	B	301	CYS
1	B	311	ILE
1	B	336	ARG
1	B	343	ARG
1	B	375	ILE
1	B	377	ASN
1	B	385	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	389	ILE
1	B	392	LYS
1	B	397	ILE
1	B	420	ASN
1	B	473	SER
1	B	479	LEU
1	B	486	VAL
1	B	489	LYS
1	B	500	LEU
1	B	507	VAL
1	B	514	LEU
1	B	515	ASP
1	B	543	LEU
1	B	558	VAL
1	B	562	ASN
1	B	594	ILE
1	B	600	THR
1	B	619	VAL
1	B	621	ASN
1	B	627	TRP
1	B	677	GLU
1	B	680	LEU
1	B	684	ARG
1	B	696	LYS
1	B	715	GLN
1	B	726	VAL
1	B	731	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	100	HIS
1	A	169	ASN
1	A	227	GLN
1	A	229	ASN
1	A	263	ASN
1	A	420	ASN
1	A	435	GLN
1	A	455	GLN
1	A	483	HIS
1	A	508	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	572	ASN
1	A	586	GLN
1	A	592	HIS
1	A	621	ASN
1	A	679	ASN
1	A	715	GLN
1	A	750	HIS
1	B	72	GLN
1	B	103	ASN
1	B	123	GLN
1	B	126	HIS
1	B	169	ASN
1	B	229	ASN
1	B	263	ASN
1	B	298	HIS
1	B	377	ASN
1	B	420	ASN
1	B	469	GLN
1	B	483	HIS
1	B	562	ASN
1	B	586	GLN
1	B	606	GLN
1	B	621	ASN
1	B	679	ASN
1	B	682	HIS
1	B	715	GLN
1	B	749	GLN
1	B	750	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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
2	NAG	A	796	-	14,14,15	0.50	0	17,19,21	0.96	0
2	NAG	B	794	1	14,14,15	0.58	0	17,19,21	0.82	0
3	B1Q	B	1	-	29,30,30	0.73	0	35,44,44	1.62	8 (22%)
2	NAG	A	794	-	14,14,15	0.53	0	17,19,21	0.85	1 (5%)
3	B1Q	A	1	-	29,30,30	0.70	0	35,44,44	1.70	10 (28%)
2	NAG	B	796	-	14,14,15	0.53	0	17,19,21	1.30	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	796	-	-	0/6/23/26	0/1/1/1
2	NAG	B	794	1	-	0/6/23/26	0/1/1/1
3	B1Q	B	1	-	-	2/10/47/47	0/4/4/4
2	NAG	A	794	-	-	2/6/23/26	0/1/1/1
3	B1Q	A	1	-	-	2/10/47/47	0/4/4/4
2	NAG	B	796	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	B1Q	C27-O22-C12	4.68	124.37	117.51
3	B	1	B1Q	C26-O23-C15	4.22	123.70	117.51
3	A	1	B1Q	O23-C15-C12	3.68	120.39	115.40
3	A	1	B1Q	C7-C2-N1	-3.28	109.15	116.18
3	B	1	B1Q	O23-C15-C12	3.22	119.78	115.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	B1Q	C27-O22-C12	3.16	122.15	117.51
3	A	1	B1Q	C26-O23-C15	2.98	121.89	117.51
3	B	1	B1Q	O22-C12-C15	2.79	119.19	115.40
3	B	1	B1Q	C7-C2-N1	-2.77	110.24	116.18
2	B	796	NAG	C3-C4-C5	2.77	115.25	110.23
3	A	1	B1Q	C2-C7-N3	-2.56	107.08	111.45
3	A	1	B1Q	O19-C5-N1	2.48	127.64	124.87
2	B	796	NAG	C1-O5-C5	-2.48	108.86	112.19
3	B	1	B1Q	O19-C5-C16	-2.41	123.76	127.28
3	A	1	B1Q	C13-N1-C2	-2.32	119.41	122.84
3	B	1	B1Q	O19-C5-N1	2.30	127.44	124.87
3	A	1	B1Q	O19-C5-C16	-2.18	124.09	127.28
3	B	1	B1Q	O22-C12-C11	-2.16	120.36	124.08
3	A	1	B1Q	O23-C15-C14	-2.12	120.42	124.08
2	A	794	NAG	C2-N2-C7	2.11	125.72	122.90
2	B	796	NAG	C2-N2-C7	-2.06	120.14	122.90
3	A	1	B1Q	O22-C12-C15	2.02	118.15	115.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	B1Q	C13-C18-C25-F24
3	B	1	B1Q	C15-C12-O22-C27
2	A	794	NAG	C8-C7-N2-C2
3	B	1	B1Q	C11-C12-O22-C27
2	A	794	NAG	O7-C7-N2-C2
3	A	1	B1Q	C12-C15-O23-C26

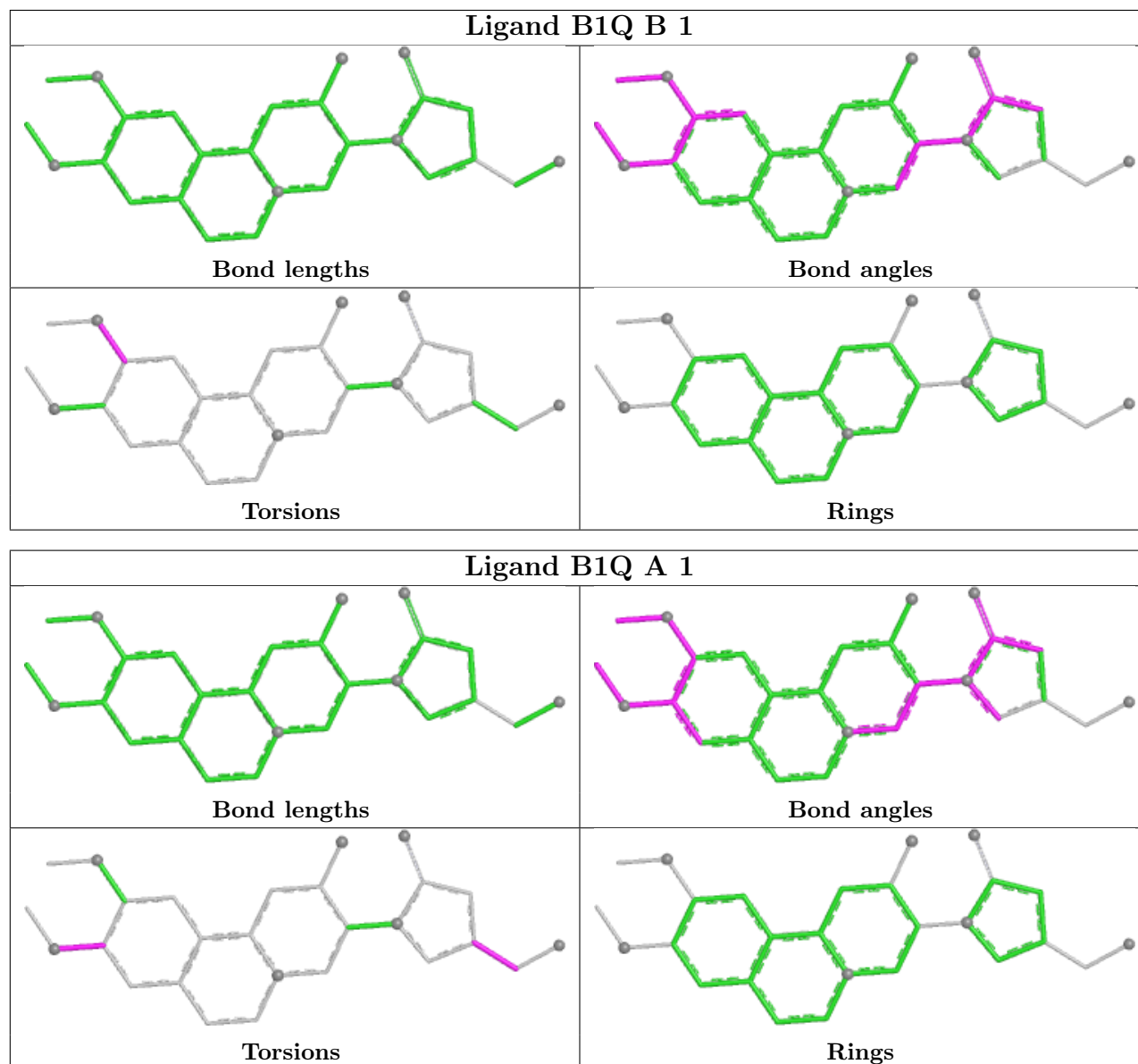
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	796	NAG	3	0
2	A	794	NAG	3	0
2	B	796	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	728/728 (100%)	-0.30	5 (0%) 84 81	25, 39, 59, 73	0
1	B	728/728 (100%)	-0.26	4 (0%) 87 85	25, 39, 57, 72	0
All	All	1456/1456 (100%)	-0.28	9 (0%) 85 83	25, 39, 59, 73	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	3.3
1	B	766	PRO	3.0
1	B	143	ILE	2.8
1	A	39	SER	2.7
1	A	278	SER	2.6
1	B	110	ASP	2.6
1	A	378	GLU	2.4
1	A	105	TYR	2.3
1	A	452	GLU	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,

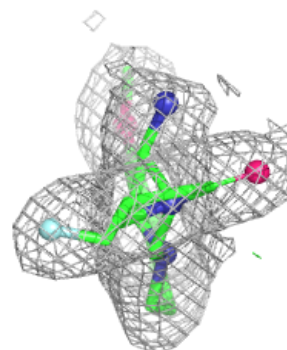
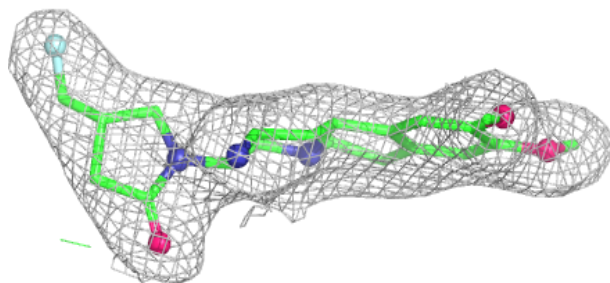
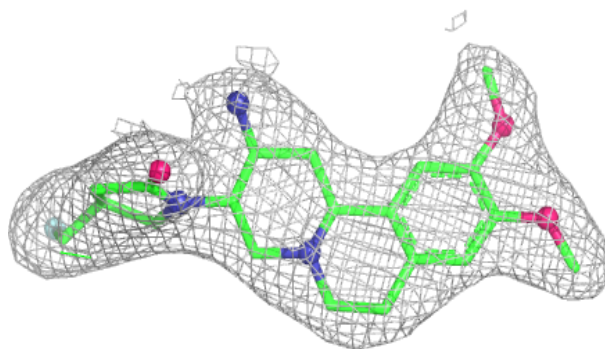
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

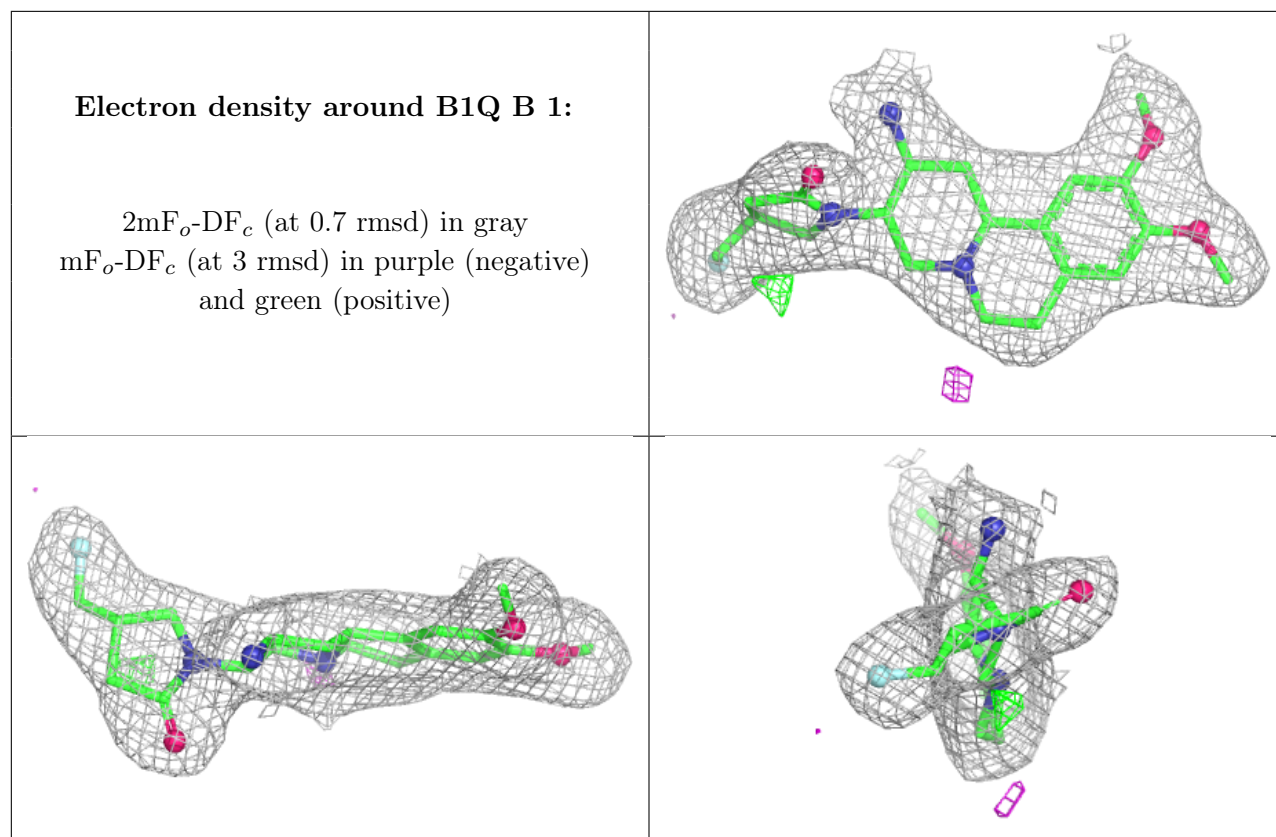
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	796	14/15	0.82	0.12	44,50,53,53	0
2	NAG	B	796	14/15	0.87	0.10	49,54,55,55	0
2	NAG	A	794	14/15	0.91	0.09	46,48,50,50	0
2	NAG	B	794	14/15	0.94	0.08	41,43,46,46	0
3	B1Q	A	1	27/27	0.95	0.07	24,28,30,31	0
3	B1Q	B	1	27/27	0.96	0.06	24,28,29,30	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 B1Q A 1:

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.