



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:21 AM UTC

PDB ID : 3KWJ / pdb_00003kwj
Title : Structure of human DPP-IV with (2S,3S,11bS)-3-(3-Fluoromethyl-phenyl)-9,10-dimethoxy-1,3,4,6,7,11b-hexahydro-2H-pyrido[2,1-a]isoquinolin-2-ylamine
Authors : Hennig, M.; Stihle, M.; Thoma, R.
Deposited on : 2009-12-01
Resolution : 2.80 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

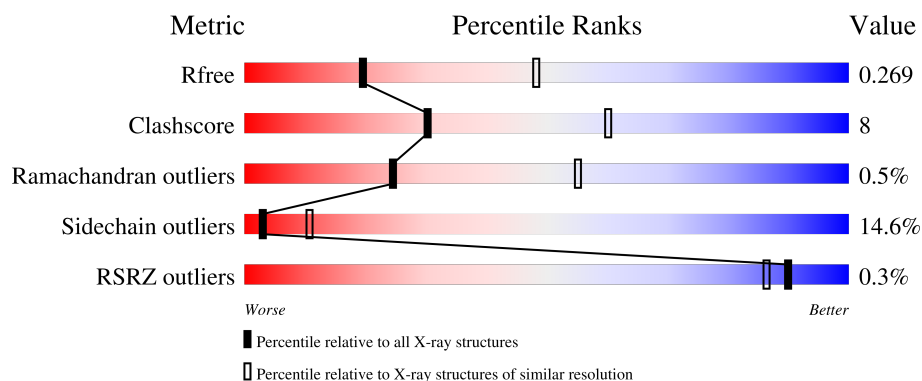
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	
1	B	728	

2 Entry composition [i](#)

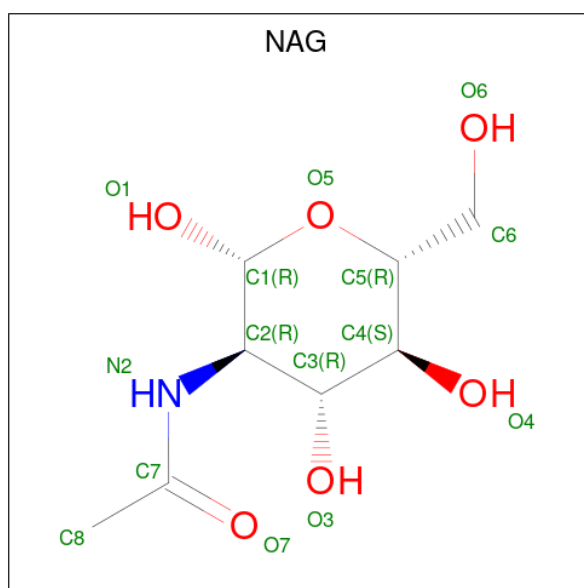
There are 4 unique types of molecules in this entry. The entry contains 12060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 soluble form.

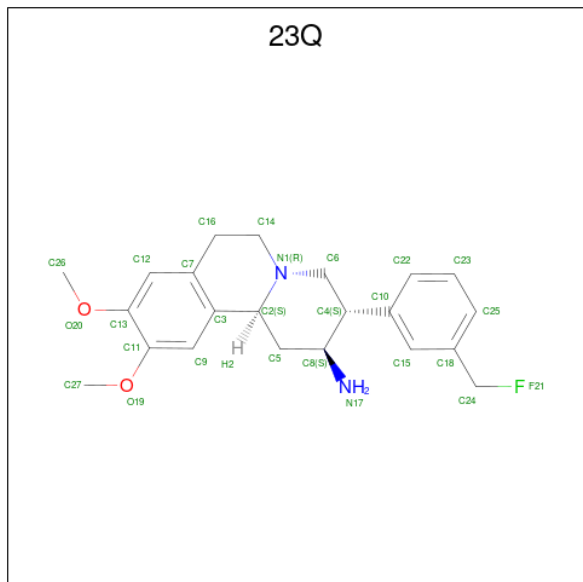
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- 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 (2S,3S,11bS)-3-[3-(fluoromethyl)phenyl]-9,10-dimethoxy-1,3,4,6,7,11b-hexahydro-2H-pyrido[2,1-a]isoquinolin-2-amine (CCD ID: 23Q) (formula: C₂₂H₂₇FN₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			27	22	1	2	2		
3	B	1	Total	C	F	N	O	0	0
			27	22	1	2	2		

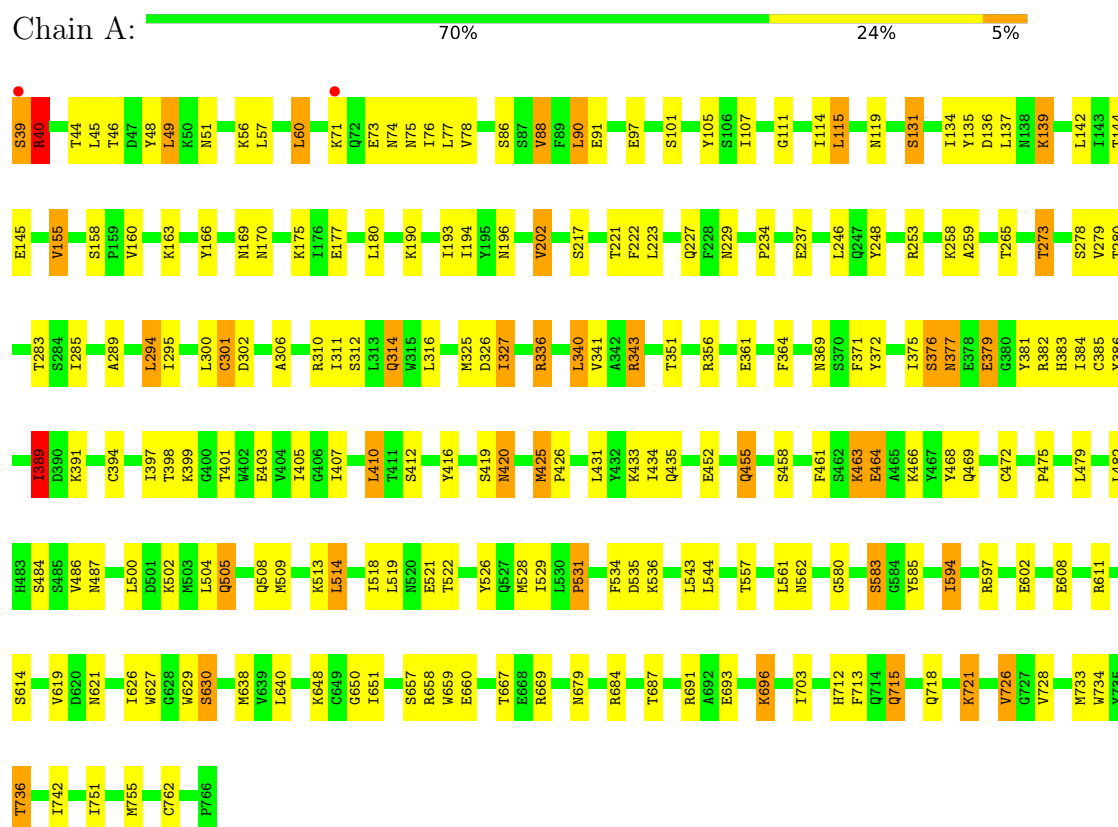
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	15	Total	O	0	0
			15	15		

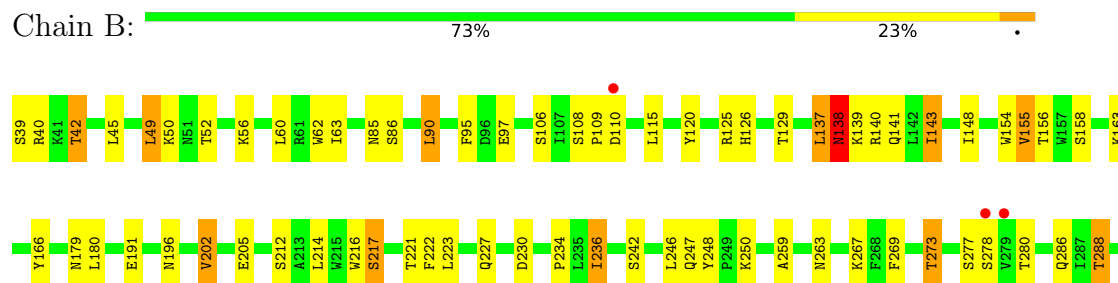
3 Residue-property plots

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: Dipeptidyl peptidase 4 soluble form



- Molecule 1: Dipeptidyl peptidase 4 soluble form



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.20Å 68.96Å 421.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (15.00-2.80) 93.3 (15.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.276 0.225 , 0.269	Depositor DCC
R_{free} test set	2320 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12060	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, 23Q

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	0.63	0/6135	0.94	6/8344 (0.1%)
1	B	0.69	0/6135	0.97	4/8344 (0.0%)
All	All	0.66	0/12270	0.96	10/16688 (0.1%)

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	B	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	389	ILE	N-CA-C	6.22	116.40	110.42
1	A	202	VAL	CB-CA-C	-5.91	104.40	111.97
1	A	139	LYS	N-CA-C	-5.83	102.84	110.53
1	A	389	ILE	N-CA-C	5.73	117.16	110.62
1	A	630	SER	CB-CA-C	-5.68	110.05	116.63
1	B	141	GLN	N-CA-C	5.50	118.44	109.59
1	A	40	ARG	N-CA-C	5.41	122.33	110.80
1	A	531	PRO	O-C-N	5.38	123.68	121.15
1	B	202	VAL	CB-CA-C	-5.35	103.87	112.16
1	B	148	ILE	N-CA-C	-5.25	104.14	109.02

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	110	ASP	Peptide

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	5684	98	0
1	B	5963	0	5684	107	0
2	A	28	0	26	2	0
2	B	28	0	26	3	0
3	A	27	0	27	0	0
3	B	27	0	27	1	0
4	A	9	0	0	1	0
4	B	15	0	0	0	0
All	All	12060	0	11474	198	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 8.

All (198) 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:229:ASN:HD21	2:A:796:NAG:C1	1.27	1.44
1:B:85:ASN:HD21	2:B:794:NAG:C1	1.45	1.29
1:A:229:ASN:ND2	2:A:796:NAG:C1	2.11	1.13
1:B:85:ASN:ND2	2:B:794:NAG:C1	2.22	1.00
1:B:735:TYR:OH	1:B:750:HIS:HD2	1.47	0.96
1:B:600:THR:HG22	1:B:601:PHE:H	1.33	0.92
1:A:221:THR:O	1:A:273:THR:HB	1.69	0.92
1:B:600:THR:HG22	1:B:601:PHE:N	1.89	0.85
1:B:155:VAL:HG13	1:B:166:TYR:HB3	1.59	0.84
1:B:221:THR:O	1:B:273:THR:HB	1.78	0.83
1:A:751:ILE:HG12	1:A:755:MET:HE2	1.59	0.83
1:B:648:LYS:HE3	1:B:762:CYS:O	1.79	0.83
1:A:580:GLY:O	1:A:583:SER:OG	1.96	0.83
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.65	0.79
1:A:403:GLU:H	1:A:420:ASN:HD21	1.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASN:OD1	1:A:227:GLN:HG3	1.84	0.78
1:A:377:ASN:HD22	1:A:377:ASN:C	1.92	0.77
1:B:735:TYR:OH	1:B:750:HIS:CD2	2.36	0.76
1:B:657:SER:H	1:B:715:GLN:NE2	1.84	0.75
1:A:504:LEU:HD22	1:A:509:MET:HE2	1.69	0.73
1:A:420:ASN:H	1:A:420:ASN:HD22	1.38	0.72
1:A:455:GLN:HB2	1:A:475:PRO:HD3	1.76	0.68
1:B:562:ASN:C	1:B:562:ASN:HD22	2.02	0.68
1:B:726:VAL:HG12	1:B:728:VAL:HG23	1.76	0.67
1:B:312:SER:OG	1:B:325:MET:HE3	1.95	0.66
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.77	0.65
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.79	0.64
1:B:461:PHE:CD1	1:B:468:TYR:HB3	2.33	0.64
1:B:291:ALA:O	1:B:295:ILE:HG22	1.97	0.64
1:B:600:THR:CG2	1:B:601:PHE:N	2.60	0.63
1:A:77:LEU:HD23	1:A:88:VAL:HA	1.81	0.63
1:A:463:LYS:O	1:A:464:GLU:HB2	1.98	0.63
1:B:500:LEU:HD22	1:B:504:LEU:HG	1.80	0.63
1:A:693:GLU:O	1:A:696:LYS:HG3	1.99	0.63
1:A:163:LYS:HD3	1:A:273:THR:HG21	1.81	0.62
1:B:403:GLU:H	1:B:420:ASN:HD21	1.46	0.62
1:B:137:LEU:C	1:B:139:LYS:H	2.07	0.61
1:A:312:SER:OG	1:A:325:MET:HE3	2.00	0.61
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.02	0.59
1:A:736:THR:HG21	1:B:717:ALA:O	2.01	0.59
1:B:386:TYR:HB2	1:B:397:ILE:HD13	1.84	0.59
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.85	0.59
1:B:420:ASN:H	1:B:420:ASN:HD22	1.51	0.59
1:B:377:ASN:ND2	1:B:381:TYR:H	2.01	0.59
1:A:718:GLN:OE1	1:A:721:LYS:NZ	2.36	0.59
1:B:402:TRP:NE1	1:B:421:GLU:HG3	2.16	0.58
1:B:402:TRP:CE2	1:B:421:GLU:HG3	2.39	0.58
1:B:597:ARG:O	1:B:600:THR:HB	2.03	0.57
1:B:516:PHE:CD1	1:B:523:LYS:HG2	2.39	0.57
1:B:657:SER:H	1:B:715:GLN:HE21	1.51	0.57
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.05	0.57
1:A:638:MET:O	1:A:691:ARG:NH1	2.38	0.57
1:B:543:LEU:HD12	1:B:567:LEU:HD13	1.87	0.57
1:B:648:LYS:CE	1:B:762:CYS:O	2.52	0.57
1:B:598:LEU:O	1:B:682:HIS:HE1	1.88	0.56
1:A:657:SER:H	1:A:715:GLN:NE2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:VAL:CG1	1:B:728:VAL:HG23	2.35	0.56
1:B:377:ASN:C	1:B:377:ASN:HD22	2.12	0.55
1:B:401:THR:HG22	1:B:401:THR:O	2.06	0.55
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.88	0.55
1:B:304:THR:O	1:B:312:SER:HB3	2.06	0.55
1:B:42:THR:HG23	1:B:570:THR:OG1	2.06	0.55
1:B:422:TYR:CE2	1:B:423:LYS:HD2	2.41	0.55
1:A:44:THR:HG22	1:A:46:THR:H	1.71	0.54
1:B:386:TYR:HB2	1:B:397:ILE:CD1	2.37	0.54
1:A:377:ASN:ND2	1:A:379:GLU:H	2.05	0.54
1:A:658:ARG:HG3	1:A:687:THR:HG22	1.90	0.54
1:A:594:ILE:HD11	1:A:602:GLU:OE1	2.08	0.53
1:A:289:ALA:HB3	1:A:294:LEU:HD13	1.90	0.53
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.44	0.53
1:A:514:LEU:HD12	1:A:557:THR:HG22	1.90	0.53
1:B:327:ILE:HB	1:B:343:ARG:HG3	1.91	0.53
1:A:169:ASN:O	1:A:170:ASN:HB2	2.07	0.53
1:B:544:LEU:HD23	1:B:626:ILE:HD12	1.90	0.52
1:B:580:GLY:O	1:B:583:SER:OG	2.27	0.52
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.90	0.52
1:A:416:TYR:CE2	1:A:433:LYS:HG3	2.45	0.52
1:A:461:PHE:CD1	1:A:468:TYR:HB3	2.45	0.51
1:B:384:ILE:HG13	1:B:404:VAL:HG21	1.93	0.51
1:B:461:PHE:CE1	1:B:468:TYR:HB3	2.46	0.51
1:A:76:ILE:HD12	1:A:90:LEU:HB3	1.92	0.51
1:B:594:ILE:HD11	1:B:602:GLU:H	1.75	0.51
1:A:105:TYR:HA	1:A:115:LEU:O	2.11	0.51
1:B:137:LEU:O	1:B:139:LYS:N	2.37	0.51
1:A:626:ILE:O	1:A:650:GLY:HA2	2.12	0.50
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.91	0.50
1:B:356:ARG:NH2	1:B:403:GLU:OE1	2.42	0.50
1:A:119:ASN:HB2	1:A:131:SER:HB2	1.94	0.50
1:A:509:MET:HE1	1:A:561:LEU:HD21	1.93	0.50
1:A:693:GLU:HA	1:A:726:VAL:HG11	1.94	0.50
1:B:420:ASN:H	1:B:420:ASN:ND2	2.09	0.50
1:A:258:LYS:HD2	1:B:247:GLN:HG2	1.94	0.50
1:A:651:ILE:HD13	1:A:755:MET:HG2	1.94	0.50
1:B:660:GLU:OE2	1:B:684:ARG:NH2	2.39	0.49
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.47	0.49
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.48	0.49
1:A:386:TYR:O	1:A:394:CYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:C	1:B:139:LYS:N	2.70	0.49
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.12	0.49
1:A:155:VAL:HG13	1:A:166:TYR:HB3	1.95	0.48
1:A:648:LYS:NZ	1:A:762:CYS:O	2.39	0.48
1:A:356:ARG:HD2	4:A:23:HOH:O	2.12	0.48
1:B:519:LEU:O	1:B:520:ASN:C	2.56	0.48
1:B:675:THR:C	1:B:680:LEU:HB2	2.38	0.48
1:A:659:TRP:HB3	1:A:667:THR:CG2	2.44	0.48
1:B:472:CYS:O	1:B:478:PRO:HA	2.13	0.48
1:A:403:GLU:H	1:A:420:ASN:ND2	2.06	0.48
1:A:258:LYS:HG3	1:B:248:TYR:CZ	2.48	0.48
1:B:163:LYS:NZ	1:B:273:THR:HG22	2.29	0.48
1:A:526:TYR:CD2	1:A:526:TYR:C	2.91	0.48
1:A:712:HIS:O	1:A:713:PHE:C	2.57	0.48
1:B:418:ILE:HA	1:B:430:ASN:O	2.14	0.47
1:A:364:PHE:CD1	1:A:371:PHE:HB3	2.49	0.47
1:A:703:ILE:HG12	1:A:733:MET:HB3	1.96	0.47
1:B:549:GLY:O	1:B:552:SER:HB2	2.14	0.47
1:B:62:TRP:CE3	1:B:462:SER:HB3	2.50	0.47
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.97	0.47
1:A:377:ASN:C	1:A:377:ASN:ND2	2.65	0.47
1:B:90:LEU:HD11	1:B:95:PHE:HE2	1.80	0.47
1:B:277:SER:HB3	1:B:280:THR:HB	1.97	0.46
1:B:296:GLY:O	1:B:298:HIS:HD2	1.98	0.46
1:B:614:SER:HA	1:B:619:VAL:CG2	2.45	0.46
1:B:217:SER:HB3	1:B:222:PHE:HB2	1.97	0.46
1:A:327:ILE:HB	1:A:343:ARG:HG3	1.97	0.46
1:B:85:ASN:HD21	2:B:794:NAG:C2	2.21	0.46
1:A:384:ILE:HG12	1:A:407:ILE:HD11	1.97	0.46
1:A:463:LYS:O	1:A:464:GLU:CB	2.64	0.46
1:A:60:LEU:HD11	1:A:469:GLN:CD	2.41	0.46
1:A:416:TYR:HE2	1:A:433:LYS:HG3	1.81	0.46
1:A:531:PRO:HD2	1:A:534:PHE:HD1	1.81	0.46
1:B:310:ARG:NH2	1:B:368:GLY:O	2.49	0.45
1:B:640:LEU:HD11	1:B:650:GLY:CA	2.46	0.45
1:B:485:SER:O	1:B:486:VAL:C	2.59	0.45
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.97	0.45
1:A:627:TRP:HB2	1:A:651:ILE:HB	1.98	0.45
1:A:217:SER:HB3	1:A:222:PHE:HB2	1.98	0.45
1:A:611:ARG:O	1:A:614:SER:HB2	2.15	0.45
1:A:629:TRP:HZ2	1:A:742:ILE:HG13	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLU:OE2	3:B:1:23Q:N17	2.49	0.45
1:B:509:MET:HE3	1:B:510:PRO:HD2	1.99	0.45
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.51	0.44
1:A:504:LEU:HD13	1:A:509:MET:HE2	1.99	0.44
1:B:109:PRO:HG2	1:B:158:SER:O	2.16	0.44
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.98	0.44
1:B:459:VAL:HG22	1:B:460:SER:N	2.32	0.44
1:A:136:ASP:O	1:A:139:LYS:O	2.35	0.44
1:A:259:ALA:HB3	1:A:660:GLU:HA	1.99	0.44
1:B:143:ILE:HD13	1:B:179:ASN:HA	2.00	0.44
1:A:340:LEU:HB2	1:A:343:ARG:HD2	1.99	0.44
1:A:659:TRP:HB3	1:A:667:THR:HG21	1.99	0.44
1:A:696:LYS:HG3	1:A:696:LYS:H	1.62	0.44
1:A:703:ILE:HA	1:A:733:MET:O	2.18	0.44
1:A:728:VAL:O	1:B:750:HIS:HE1	2.01	0.44
1:B:158:SER:HA	1:B:216:TRP:CD1	2.53	0.44
1:B:288:THR:HG23	1:B:294:LEU:HD11	2.00	0.43
1:A:369:ASN:O	1:A:389:ILE:HB	2.18	0.43
1:A:375:ILE:HG22	1:A:376:SER:O	2.18	0.43
1:B:481:THR:OG1	1:B:483:HIS:HE1	2.00	0.43
1:A:39:SER:HB3	1:A:505:GLN:O	2.19	0.43
1:B:319:ILE:C	1:B:321:ASN:H	2.26	0.43
1:A:425:MET:HA	1:A:426:PRO:HD3	1.83	0.43
1:B:138:ASN:O	1:B:139:LYS:HG3	2.19	0.43
1:B:414:TYR:HA	1:B:434:ILE:O	2.19	0.43
1:A:594:ILE:HD12	1:A:594:ILE:HA	1.80	0.43
1:A:306:ALA:HB3	1:A:310:ARG:HB3	2.02	0.42
1:B:236:ILE:HD12	1:B:712:HIS:CD2	2.54	0.42
1:B:471:ARG:HG3	1:B:480:TYR:CE2	2.54	0.42
1:B:125:ARG:HD2	1:B:126:HIS:CE1	2.54	0.42
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.49	0.42
1:A:301:CYS:HB3	1:A:314:GLN:HB3	2.01	0.42
1:B:377:ASN:HD21	1:B:381:TYR:H	1.67	0.42
1:B:434:ILE:HG12	1:B:442:VAL:HG22	2.01	0.42
1:A:383:HIS:HB3	1:A:398:THR:OG1	2.20	0.42
1:A:381:TYR:CZ	1:A:401:THR:HG23	2.55	0.42
1:A:372:TYR:CE1	1:A:410:LEU:HD11	2.54	0.41
1:B:455:GLN:HB2	1:B:475:PRO:HD3	2.01	0.41
1:A:40:ARG:HD3	1:A:40:ARG:HA	1.45	0.41
1:A:177:GLU:HB2	1:A:180:LEU:HB2	2.03	0.41
1:B:106:SER:HB3	1:B:115:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.50	0.41
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.20	0.41
1:A:234:PRO:HB2	1:B:248:TYR:CE2	2.56	0.41
1:B:269:PHE:CE1	1:B:286:GLN:HB2	2.56	0.41
1:A:48:TYR:CD1	1:A:562:ASN:HA	2.55	0.41
1:B:431:LEU:HD13	1:B:459:VAL:HG11	2.03	0.41
1:B:684:ARG:O	1:B:687:THR:HG23	2.21	0.41
1:A:734:TRP:CD1	1:A:734:TRP:C	2.99	0.41
1:B:534:PHE:HZ	1:B:618:PHE:CD1	2.38	0.41
1:A:519:LEU:HD23	1:A:519:LEU:HA	1.81	0.41
1:B:742:ILE:HG22	1:B:742:ILE:O	2.20	0.41
1:A:45:LEU:HG	1:A:49:LEU:HD22	2.03	0.41
1:B:259:ALA:HB3	1:B:660:GLU:HA	2.02	0.41
1:B:415:LEU:C	1:B:415:LEU:HD23	2.46	0.41
1:B:644:SER:C	1:B:646:VAL:H	2.29	0.41
1:A:285:ILE:HG21	1:A:336:ARG:HA	2.03	0.40
1:A:535:ASP:C	1:A:535:ASP:OD1	2.63	0.40
1:B:481:THR:CB	1:B:483:HIS:HE1	2.35	0.40
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.98	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	726/728 (100%)	671 (92%)	50 (7%)	5 (1%)	18	47
1	B	726/728 (100%)	686 (94%)	38 (5%)	2 (0%)	36	66
All	All	1452/1456 (100%)	1357 (94%)	88 (6%)	7 (0%)	24	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	464	GLU
1	B	138	ASN
1	A	73	GLU
1	A	111	GLY
1	B	242	SER
1	A	486	VAL

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	653/653 (100%)	543 (83%)	110 (17%)	2	8
1	B	653/653 (100%)	572 (88%)	81 (12%)	4	16
All	All	1306/1306 (100%)	1115 (85%)	191 (15%)	3	11

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	40	ARG
1	A	49	LEU
1	A	51	ASN
1	A	56	LYS
1	A	57	LEU
1	A	60	LEU
1	A	71	LYS
1	A	74	ASN
1	A	75	ASN
1	A	78	VAL
1	A	86	SER
1	A	88	VAL
1	A	90	LEU
1	A	91	GLU
1	A	97	GLU
1	A	101	SER

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Mol	Chain	Res	Type
1	A	107	ILE
1	A	115	LEU
1	A	131	SER
1	A	134	ILE
1	A	137	LEU
1	A	142	LEU
1	A	144	THR
1	A	145	GLU
1	A	155	VAL
1	A	158	SER
1	A	160	VAL
1	A	175	LYS
1	A	190	LYS
1	A	202	VAL
1	A	223	LEU
1	A	246	LEU
1	A	273	THR
1	A	278	SER
1	A	279	VAL
1	A	280	THR
1	A	283	THR
1	A	294	LEU
1	A	295	ILE
1	A	300	LEU
1	A	301	CYS
1	A	311	ILE
1	A	314	GLN
1	A	316	LEU
1	A	326	ASP
1	A	327	ILE
1	A	336	ARG
1	A	340	LEU
1	A	341	VAL
1	A	343	ARG
1	A	351	THR
1	A	361	GLU
1	A	376	SER
1	A	377	ASN
1	A	379	GLU
1	A	382	ARG
1	A	385	CYS
1	A	389	ILE

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Mol	Chain	Res	Type
1	A	391	LYS
1	A	397	ILE
1	A	399	LYS
1	A	405	ILE
1	A	410	LEU
1	A	412	SER
1	A	419	SER
1	A	420	ASN
1	A	425	MET
1	A	431	LEU
1	A	434	ILE
1	A	435	GLN
1	A	452	GLU
1	A	455	GLN
1	A	458	SER
1	A	463	LYS
1	A	466	LYS
1	A	472	CYS
1	A	479	LEU
1	A	482	LEU
1	A	484	SER
1	A	487	ASN
1	A	500	LEU
1	A	502	LYS
1	A	505	GLN
1	A	508	GLN
1	A	513	LYS
1	A	514	LEU
1	A	518	ILE
1	A	521	GLU
1	A	522	THR
1	A	528	MET
1	A	529	ILE
1	A	536	LYS
1	A	543	LEU
1	A	544	LEU
1	A	583	SER
1	A	594	ILE
1	A	597	ARG
1	A	608	GLU
1	A	619	VAL
1	A	621	ASN

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Mol	Chain	Res	Type
1	A	630	SER
1	A	669	ARG
1	A	679	ASN
1	A	684	ARG
1	A	696	LYS
1	A	715	GLN
1	A	721	LYS
1	A	726	VAL
1	A	736	THR
1	B	39	SER
1	B	40	ARG
1	B	42	THR
1	B	49	LEU
1	B	50	LYS
1	B	52	THR
1	B	56	LYS
1	B	60	LEU
1	B	63	ILE
1	B	86	SER
1	B	90	LEU
1	B	97	GLU
1	B	108	SER
1	B	120	TYR
1	B	129	THR
1	B	137	LEU
1	B	138	ASN
1	B	140	ARG
1	B	143	ILE
1	B	155	VAL
1	B	156	THR
1	B	180	LEU
1	B	191	GLU
1	B	202	VAL
1	B	214	LEU
1	B	217	SER
1	B	223	LEU
1	B	230	ASP
1	B	236	ILE
1	B	246	LEU
1	B	250	LYS
1	B	263	ASN
1	B	267	LYS

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Mol	Chain	Res	Type
1	B	273	THR
1	B	278	SER
1	B	288	THR
1	B	295	ILE
1	B	300	LEU
1	B	311	ILE
1	B	326	ASP
1	B	332	GLU
1	B	336	ARG
1	B	340	LEU
1	B	343	ARG
1	B	361	GLU
1	B	375	ILE
1	B	377	ASN
1	B	385	CYS
1	B	389	ILE
1	B	392	LYS
1	B	397	ILE
1	B	420	ASN
1	B	452	GLU
1	B	466	LYS
1	B	479	LEU
1	B	489	LYS
1	B	498	SER
1	B	500	LEU
1	B	505	GLN
1	B	507	VAL
1	B	514	LEU
1	B	536	LYS
1	B	538	LYS
1	B	543	LEU
1	B	552	SER
1	B	558	VAL
1	B	562	ASN
1	B	594	ILE
1	B	597	ARG
1	B	600	THR
1	B	614	SER
1	B	619	VAL
1	B	677	GLU
1	B	679	ASN
1	B	680	LEU

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Mol	Chain	Res	Type
1	B	684	ARG
1	B	715	GLN
1	B	726	VAL
1	B	731	GLN
1	B	759	ILE
1	B	764	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	103	ASN
1	A	162	HIS
1	A	169	ASN
1	A	227	GLN
1	A	229	ASN
1	A	247	GLN
1	A	263	ASN
1	A	377	ASN
1	A	420	ASN
1	A	430	ASN
1	A	435	GLN
1	A	483	HIS
1	A	508	GLN
1	A	586	GLN
1	A	606	GLN
1	A	621	ASN
1	A	679	ASN
1	A	715	GLN
1	A	748	HIS
1	A	749	GLN
1	B	51	ASN
1	B	85	ASN
1	B	103	ASN
1	B	126	HIS
1	B	263	ASN
1	B	298	HIS
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	430	ASN
1	B	455	GLN

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Mol	Chain	Res	Type
1	B	483	HIS
1	B	562	ASN
1	B	586	GLN
1	B	679	ASN
1	B	682	HIS
1	B	715	GLN
1	B	750	HIS
1	B	757	HIS

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](#)

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	$\# Z > 2$
3	23Q	B	1	-	28,30,30	0.96	1 (3%)	35,43,43	1.86	9 (25%)
2	NAG	A	796	-	14,14,15	0.60	0	17,19,21	0.83	0
2	NAG	B	796	1	14,14,15	0.55	0	17,19,21	1.16	2 (11%)
2	NAG	B	794	-	14,14,15	0.62	0	17,19,21	1.06	1 (5%)
3	23Q	A	1	-	28,30,30	0.97	1 (3%)	35,43,43	1.92	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	794	1	14,14,15	0.52	0	17,19,21	1.53	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
3	23Q	B	1	-	-	0/8/35/35	0/4/4/4
2	NAG	A	796	-	-	3/6/23/26	0/1/1/1
2	NAG	B	796	1	-	0/6/23/26	0/1/1/1
2	NAG	B	794	-	-	2/6/23/26	0/1/1/1
3	23Q	A	1	-	-	2/8/35/35	0/4/4/4
2	NAG	A	794	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	23Q	C10-C4	-2.47	1.48	1.51
3	B	1	23Q	C12-C13	2.23	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	23Q	C6-N1-C2	5.63	118.33	110.12
3	A	1	23Q	C26-O20-C13	5.15	125.06	117.51
3	B	1	23Q	C26-O20-C13	4.77	124.51	117.51
3	B	1	23Q	C6-N1-C2	4.69	116.96	110.12
3	B	1	23Q	O19-C11-C13	4.15	121.04	115.40
2	A	794	NAG	O5-C1-C2	-3.58	105.75	111.29
3	A	1	23Q	C27-O19-C11	3.47	122.60	117.51
3	A	1	23Q	C5-C8-C4	-3.03	107.15	111.45
2	B	796	NAG	C1-O5-C5	3.02	116.23	112.19
2	A	794	NAG	C2-N2-C7	-2.88	119.03	122.90
3	B	1	23Q	C27-O19-C11	2.77	121.58	117.51
3	A	1	23Q	O19-C11-C13	2.77	119.16	115.40
2	B	794	NAG	O5-C1-C2	-2.69	107.13	111.29
3	B	1	23Q	C9-C3-C7	-2.66	116.49	119.39
3	A	1	23Q	C5-C2-C3	-2.60	109.37	113.07
3	B	1	23Q	O19-C11-C9	-2.53	119.72	124.08
3	B	1	23Q	C14-N1-C6	2.41	114.95	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	794	NAG	O5-C5-C6	2.35	112.23	107.66
2	B	796	NAG	O5-C1-C2	-2.25	107.81	111.29
3	B	1	23Q	C11-C9-C3	2.24	124.19	119.44
3	B	1	23Q	O20-C13-C11	2.11	118.27	115.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

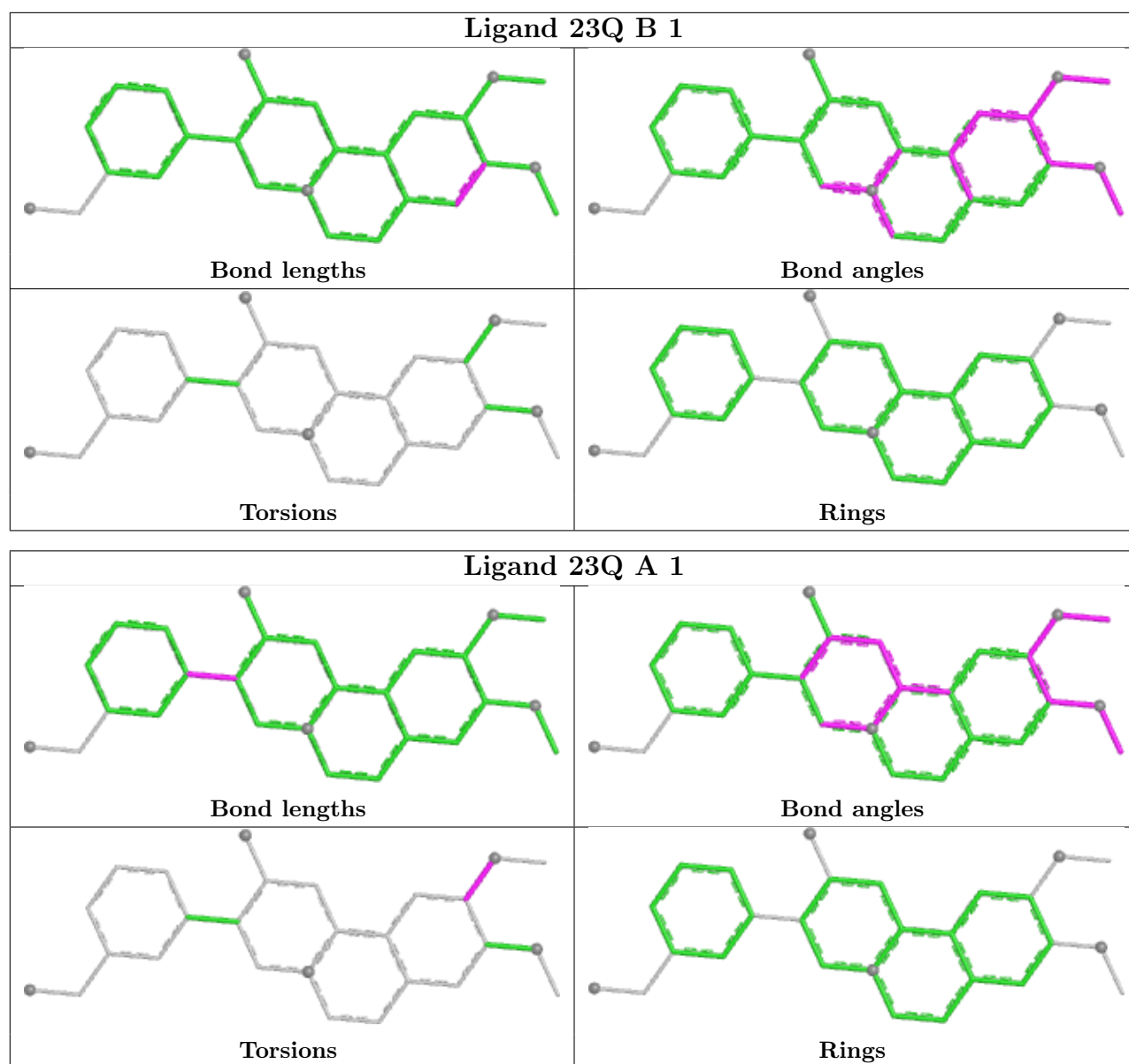
Mol	Chain	Res	Type	Atoms
3	A	1	23Q	C13-C11-O19-C27
2	B	794	NAG	O5-C5-C6-O6
2	B	794	NAG	C4-C5-C6-O6
3	A	1	23Q	C9-C11-O19-C27
2	A	794	NAG	O5-C5-C6-O6
2	A	796	NAG	O5-C5-C6-O6
2	A	796	NAG	C8-C7-N2-C2
2	A	794	NAG	C4-C5-C6-O6
2	A	796	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	23Q	1	0
2	A	796	NAG	2	0
2	B	794	NAG	3	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 [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%)	-0.15	2 (0%) 90 86	36, 56, 77, 91	0
1	B	728/728 (100%)	-0.42	3 (0%) 88 84	26, 44, 64, 80	0
All	All	1456/1456 (100%)	-0.29	5 (0%) 90 86	26, 50, 72, 91	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	110	ASP	2.8
1	B	279	VAL	2.4
1	A	39	SER	2.3
1	A	71	LYS	2.3
1	B	278	SER	2.2

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](#)

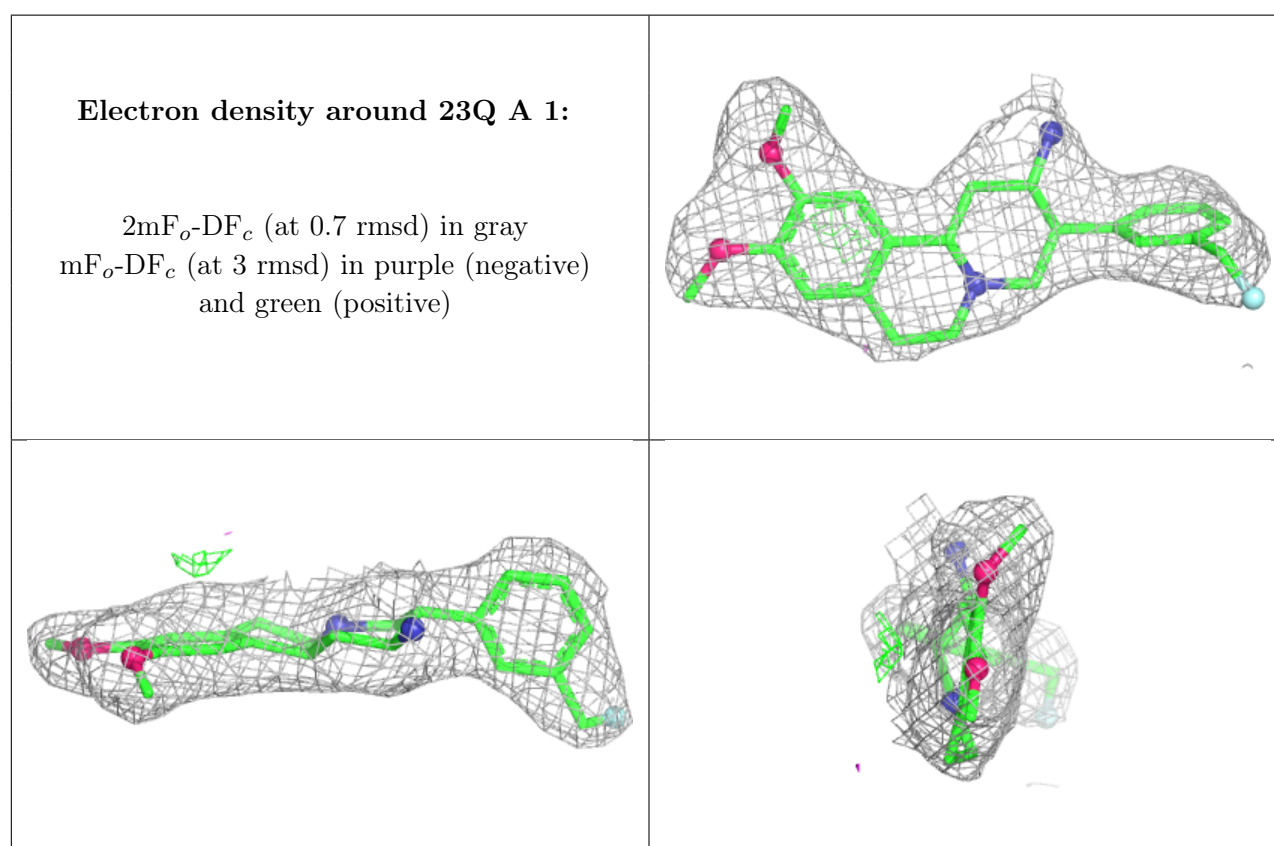
There are no oligosaccharides in this entry.

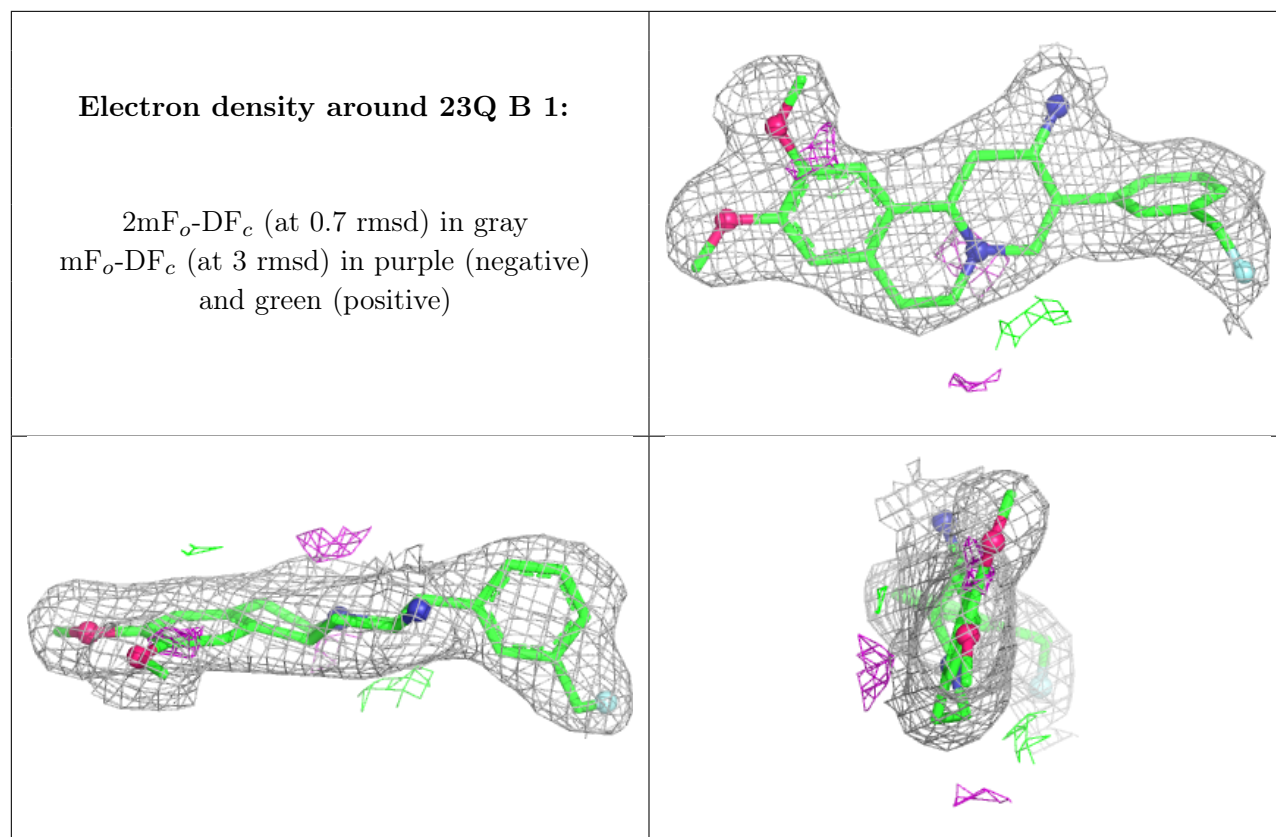
6.4 Ligands [i](#)

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	794	14/15	0.80	0.10	73,74,75,75	0
2	NAG	A	796	14/15	0.84	0.11	55,62,63,63	0
2	NAG	B	794	14/15	0.90	0.08	49,50,53,54	0
2	NAG	B	796	14/15	0.90	0.08	49,53,56,58	0
3	23Q	A	1	27/27	0.91	0.09	35,39,41,45	0
3	23Q	B	1	27/27	0.94	0.07	26,29,33,38	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.