



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:24 PM UTC

PDB ID : 4PF9 / pdb_00004pf9
Title : Crystal structure of insulin degrading enzyme complexed with inhibitor
Authors : Wang, Y.; Guo, S.
Deposited on : 2014-04-28
Resolution : 2.50 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

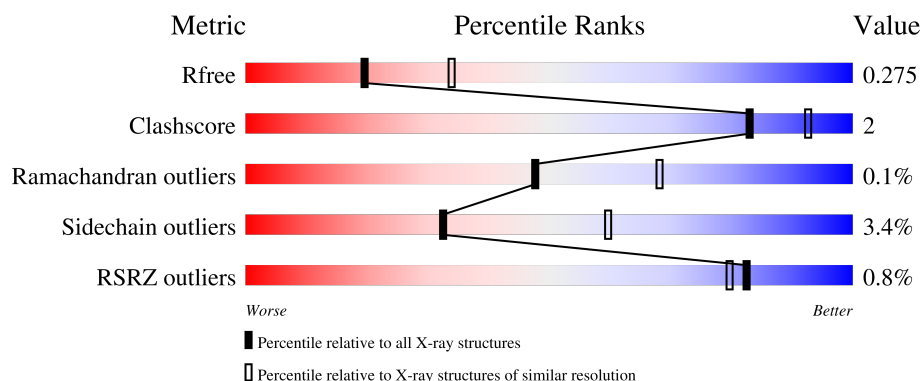
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	989	86% 10% ..
1	B	989	86% 11% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16127 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	959	Total	C	N	O	S	0	1	0
			7848	5054	1317	1455	22			
1	B	956	Total	C	N	O	S	0	0	0
			7821	5038	1313	1448	22			

There are 50 discrepancies between the modelled and reference sequences:

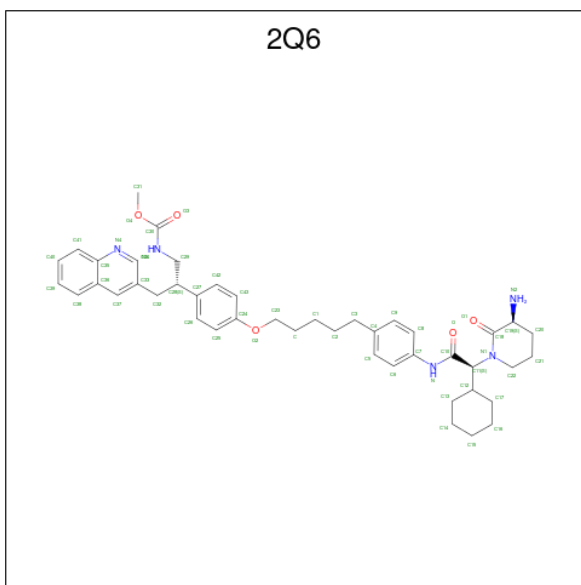
Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP P14735
A	32	GLY	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	HIS	-	expression tag	UNP P14735
A	38	HIS	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ARG	-	expression tag	UNP P14735
A	41	ALA	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	MET	-	initiating methionine	UNP P14735
B	32	GLY	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	HIS	-	expression tag	UNP P14735
B	38	HIS	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ARG	-	expression tag	UNP P14735
B	41	ALA	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is methyl [(2S)-2-[4-({5-[4-({(2S)-2-[(3S)-3-amino-2-oxopiperidin-1-yl]-2-cyclohexylacetyl}amino)phenyl]pentyl}oxy)phenyl]-3-(quinolin-3-yl)propyl]carbamate (CCD ID: 2Q6) (formula: C₄₄H₅₅N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			54	44	5	5		
2	B	1	Total	C	N	O	0	0
			54	44	5	5		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

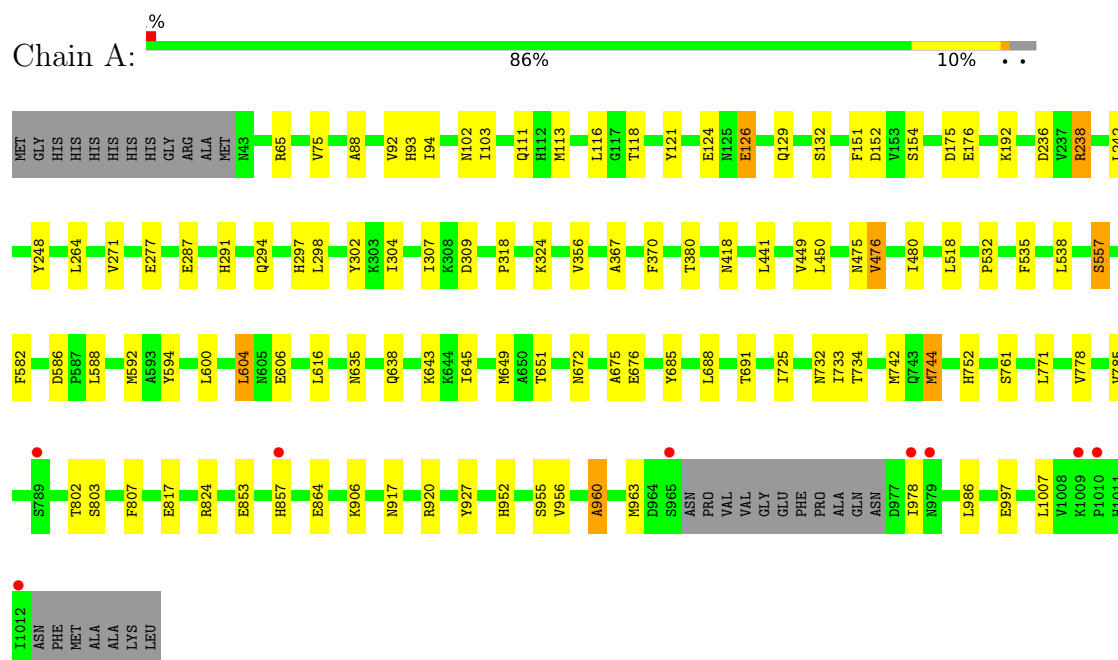
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	171	Total	O	0	0
			171	171		
4	B	177	Total	O	0	0
			177	177		

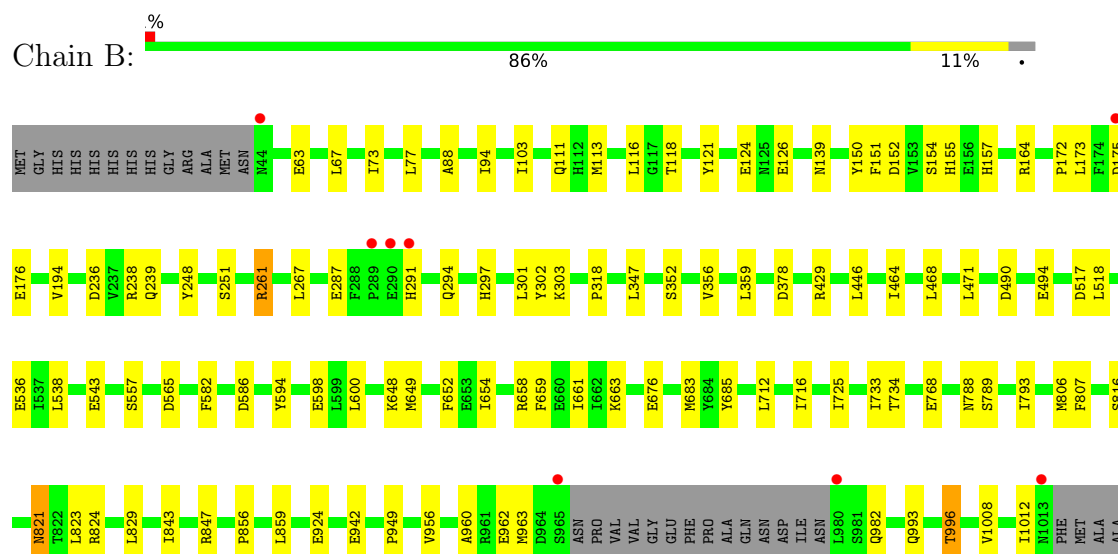
3 Residue-property plots

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: Insulin-degrading enzyme



• Molecule 1: Insulin-degrading enzyme



LYS
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.25Å 116.42Å 124.47Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.99-2.50) 99.0 (19.99-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.50Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.195 , 0.253 0.206 , 0.275	Depositor DCC
R_{free} test set	1047 reflections (1.35%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.2	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	0.94	EDS
Total number of atoms	16127	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2Q6, ZN

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	0.81	0/8046	1.34	23/10884 (0.2%)
1	B	0.81	1/8016 (0.0%)	1.35	19/10843 (0.2%)
All	All	0.81	1/16062 (0.0%)	1.34	42/21727 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	716	ILE	CA-C	5.82	1.58	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ASP	CA-CB-CG	7.59	120.19	112.60
1	B	152	ASP	CA-CB-CG	7.46	120.06	112.60
1	B	807	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	582	PHE	CA-CB-CG	-6.74	107.06	113.80
1	B	565	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	807	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	688	LEU	CA-C-N	5.98	128.22	120.44
1	A	688	LEU	C-N-CA	5.98	128.22	120.44
1	A	380	THR	N-CA-C	-5.88	102.94	110.53
1	A	418	ASN	CA-CB-CG	5.81	118.41	112.60
1	B	517	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	490	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	676	GLU	CB-CG-CD	5.66	122.22	112.60
1	A	853	GLU	N-CA-C	-5.61	106.61	113.50
1	A	307	ILE	N-CA-C	-5.55	106.29	111.45
1	B	536	GLU	CB-CG-CD	5.47	121.89	112.60
1	A	557	SER	N-CA-C	5.46	118.09	108.75
1	A	586	ASP	CA-CB-CG	5.45	118.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	962	GLU	CA-C-N	5.36	128.45	120.90
1	B	962	GLU	C-N-CA	5.36	128.45	120.90
1	A	476	VAL	CA-C-N	5.35	130.32	122.77
1	A	476	VAL	C-N-CA	5.35	130.32	122.77
1	A	691	THR	CA-C-N	5.34	127.75	120.54
1	A	691	THR	C-N-CA	5.34	127.75	120.54
1	B	582	PHE	CA-CB-CG	-5.25	108.55	113.80
1	B	821	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	594	TYR	CA-C-N	5.22	127.28	120.28
1	A	594	TYR	C-N-CA	5.22	127.28	120.28
1	B	494	GLU	N-CA-C	5.21	117.04	111.36
1	A	126	GLU	CA-C-N	5.15	127.13	120.44
1	A	126	GLU	C-N-CA	5.15	127.13	120.44
1	A	802	THR	CA-C-N	5.14	127.43	120.44
1	A	802	THR	C-N-CA	5.14	127.43	120.44
1	B	164	ARG	CA-C-N	5.13	127.11	120.44
1	B	164	ARG	C-N-CA	5.13	127.11	120.44
1	B	378	ASP	N-CA-C	-5.13	102.86	110.46
1	B	175	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	960	ALA	CA-C-N	5.08	127.40	120.54
1	A	960	ALA	C-N-CA	5.08	127.40	120.54
1	B	683	MET	CA-C-N	5.08	127.09	120.28
1	B	683	MET	C-N-CA	5.08	127.09	120.28
1	B	586	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7848	0	7791	40	0
1	B	7821	0	7765	35	0
2	A	54	0	55	1	0
2	B	54	0	55	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	171	0	0	1	0
4	B	177	0	0	0	0
All	All	16127	0	15666	74	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 2.

All (74) 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:557:SER:HB2	1:A:742:MET:HE3	1.66	0.76
1:A:309:ASP:H	1:A:672:ASN:HD21	1.35	0.74
1:A:294:GLN:H	1:A:297:HIS:HD2	1.38	0.71
1:A:475:ASN:HB3	4:A:1281:HOH:O	1.89	0.71
1:A:616:LEU:HD11	1:A:638:GLN:HG3	1.78	0.66
1:A:635:ASN:HD21	1:A:732:ASN:HD22	1.48	0.61
1:A:102:ASN:HD22	1:A:103:ILE:HG13	1.66	0.59
1:A:778:VAL:HG22	1:A:955:SER:HB2	1.86	0.58
1:A:118:THR:HG23	1:A:121:TYR:H	1.71	0.56
1:A:803:SER:HA	1:A:927:TYR:CE2	2.39	0.56
1:A:864:GLU:HG3	1:A:986:LEU:HD21	1.86	0.55
1:B:538:LEU:HD13	1:B:734:THR:HG23	1.88	0.55
1:B:600:LEU:HD21	1:B:649:MET:HG2	1.89	0.54
1:B:594:TYR:CE2	1:B:598:GLU:HG3	2.43	0.54
1:A:238:ARG:O	1:A:242:LEU:HG	2.08	0.53
1:B:648:LYS:O	1:B:652:PHE:HB2	2.09	0.53
1:A:651:THR:HG23	1:A:752:HIS:HB3	1.90	0.53
1:B:113:MET:HA	1:B:116:LEU:HD12	1.91	0.53
1:B:960:ALA:HB3	1:B:963:MET:HB2	1.90	0.53
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.91	0.52
1:A:960:ALA:HB3	1:A:963:MET:HB2	1.92	0.52
1:A:557:SER:CB	1:A:742:MET:HE3	2.38	0.52
1:A:604:LEU:HD21	1:A:645:ILE:HA	1.93	0.51
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.46	0.51
1:B:176:GLU:HG2	1:B:238:ARG:HH11	1.77	0.50
1:B:236:ASP:HB3	1:B:239:GLN:HG2	1.93	0.49
1:A:176:GLU:HG2	1:A:238:ARG:HH11	1.76	0.49
1:A:132:SER:OG	1:A:817:GLU:HG3	2.12	0.48
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.95	0.48
1:A:771:LEU:HB2	1:A:952:HIS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:SER:HA	1:B:996:THR:HG21	1.96	0.47
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.50	0.47
1:A:588:LEU:HG	1:A:592:MET:HE2	1.96	0.47
1:B:302:TYR:CD1	2:B:1101:2Q6:H21	2.49	0.47
1:B:121:TYR:HB3	1:B:126:GLU:HG2	1.96	0.47
1:B:294:GLN:H	1:B:297:HIS:HD2	1.63	0.47
1:B:291:HIS:CE1	1:B:318:PRO:HB3	2.50	0.46
1:A:600:LEU:HD21	1:A:649:MET:HG2	1.97	0.46
1:A:113:MET:HA	1:A:116:LEU:HD12	1.97	0.46
1:B:301:LEU:HD21	1:B:303:LYS:HE3	1.99	0.45
1:A:302:TYR:CD1	2:A:1101:2Q6:H21	2.50	0.45
1:A:643:LYS:HA	1:A:744:MET:CE	2.46	0.45
1:B:155:HIS:HD2	1:B:261:ARG:HD3	1.81	0.45
1:B:806:MET:SD	1:B:924:GLU:HB3	2.56	0.45
1:A:309:ASP:H	1:A:672:ASN:ND2	2.08	0.45
1:B:77:LEU:HD22	1:B:267:LEU:HB3	1.98	0.44
1:A:685:TYR:HB2	1:A:956:VAL:HG11	1.99	0.44
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.99	0.44
1:A:675:ALA:HA	1:A:785:VAL:HG21	2.00	0.44
1:A:121:TYR:HB3	1:A:126:GLU:HG2	2.00	0.44
1:B:464:ILE:O	1:B:468:LEU:HB2	2.17	0.43
1:B:658:ARG:NH1	1:B:661:ILE:HG21	2.33	0.43
1:A:298:LEU:HD21	1:A:318:PRO:HG3	2.01	0.43
1:B:468:LEU:HD12	1:B:471:LEU:HD12	2.00	0.43
1:B:942:GLU:HA	1:B:949:PRO:HD2	2.01	0.43
1:A:94:ILE:HG13	1:A:248:TYR:HB3	2.01	0.43
1:B:654:ILE:HD13	1:B:712:LEU:HD23	2.00	0.43
1:B:856:PRO:HA	1:B:859:LEU:HD12	2.01	0.42
1:A:557:SER:HA	1:A:725:ILE:O	2.20	0.42
1:B:685:TYR:HB2	1:B:956:VAL:HG11	2.01	0.42
1:A:367:ALA:HB3	1:A:370:PHE:CE2	2.55	0.42
1:B:659:PHE:O	1:B:663:LYS:HB2	2.20	0.42
1:B:94:ILE:HG13	1:B:248:TYR:HB3	2.02	0.41
1:B:118:THR:HG22	1:B:172:PRO:HA	2.02	0.41
1:B:793:ILE:O	1:B:847:ARG:HA	2.20	0.41
1:A:75:VAL:HG11	1:A:271:VAL:HG11	2.01	0.41
1:B:768:GLU:HB3	1:B:843:ILE:HG13	2.03	0.41
1:B:823:LEU:HB3	1:B:829:LEU:HD12	2.02	0.41
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.55	0.41
1:A:532:PRO:HB2	1:A:535:PHE:CE2	2.56	0.41
1:B:154:SER:HB3	1:B:157:HIS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:HB2	1:A:264:LEU:HD13	2.03	0.40
1:B:347:LEU:HD13	1:B:359:LEU:HB2	2.02	0.40
1:A:917:ASN:O	1:A:920:ARG:HB2	2.22	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	956/989 (97%)	921 (96%)	34 (4%)	1 (0%)	48	68
1	B	952/989 (96%)	913 (96%)	39 (4%)	0	100	100
All	All	1908/1978 (96%)	1834 (96%)	73 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP

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	856/878 (98%)	826 (96%)	30 (4%)	32	58
1	B	852/878 (97%)	824 (97%)	28 (3%)	33	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1708/1756 (97%)	1650 (97%)	58 (3%)	32 60

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	93	HIS
1	A	111	GLN
1	A	124	GLU
1	A	129	GLN
1	A	154	SER
1	A	192	LYS
1	A	236	ASP
1	A	238	ARG
1	A	277	GLU
1	A	287	GLU
1	A	291	HIS
1	A	304	ILE
1	A	324	LYS
1	A	356	VAL
1	A	450	LEU
1	A	476	VAL
1	A	480	ILE
1	A	518	LEU
1	A	604	LEU
1	A	606	GLU
1	A	676	GLU
1	A	733	ILE
1	A	744	MET
1	A	824	ARG
1	A	857	HIS
1	A	906	LYS
1	A	978	ILE
1	A	997	GLU
1	A	1007	LEU
1	B	63	GLU
1	B	67	LEU
1	B	103	ILE
1	B	111	GLN
1	B	124	GLU
1	B	173	LEU
1	B	194	VAL

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Mol	Chain	Res	Type
1	B	261	ARG
1	B	287	GLU
1	B	352	SER
1	B	356	VAL
1	B	429	ARG
1	B	446	LEU
1	B	518	LEU
1	B	543	GLU
1	B	557	SER
1	B	725	ILE
1	B	733	ILE
1	B	788	ASN
1	B	789	SER
1	B	816	SER
1	B	821	ASN
1	B	824	ARG
1	B	982	GLN
1	B	993	GLN
1	B	996	THR
1	B	1008	VAL
1	B	1012	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	155	HIS
1	A	184	ASN
1	A	231	ASN
1	A	232	GLN
1	A	239	GLN
1	A	252	ASN
1	A	297	HIS
1	A	323	GLN
1	A	363	GLN
1	A	575	ASN
1	A	635	ASN
1	A	672	ASN
1	A	724	HIS
1	A	781	GLN
1	B	111	GLN
1	B	148	ASN

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Mol	Chain	Res	Type
1	B	155	HIS
1	B	157	HIS
1	B	231	ASN
1	B	252	ASN
1	B	297	HIS
1	B	499	GLN
1	B	605	ASN
1	B	724	HIS
1	B	752	HIS
1	B	788	ASN
1	B	883	GLN
1	B	887	GLN
1	B	982	GLN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	2Q6	A	1101	-	58,59,59	1.61	12 (20%)	75,79,79	1.80	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2Q6	B	1101	-	58,59,59	1.49	10 (17%)	75,79,79	1.68	6 (8%)

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	2Q6	A	1101	-	-	10/40/62/62	0/6/6/6
2	2Q6	B	1101	-	-	7/40/62/62	0/6/6/6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	2Q6	C11-N1	4.88	1.54	1.47
2	B	1101	2Q6	C11-N1	4.37	1.53	1.47
2	A	1101	2Q6	C34-C33	3.90	1.47	1.38
2	B	1101	2Q6	C42-C27	3.36	1.44	1.39
2	B	1101	2Q6	C34-C33	3.25	1.46	1.38
2	A	1101	2Q6	C30-N3	3.18	1.41	1.34
2	B	1101	2Q6	C30-N3	3.09	1.40	1.34
2	A	1101	2Q6	C11-C10	2.99	1.58	1.53
2	A	1101	2Q6	C43-C24	2.97	1.44	1.38
2	A	1101	2Q6	O4-C30	2.80	1.39	1.34
2	B	1101	2Q6	C18-N1	2.67	1.40	1.34
2	B	1101	2Q6	C8-C7	2.55	1.43	1.39
2	A	1101	2Q6	C18-N1	2.45	1.39	1.34
2	A	1101	2Q6	C10-N	2.37	1.41	1.35
2	A	1101	2Q6	C36-C35	2.25	1.45	1.42
2	B	1101	2Q6	C25-C24	2.21	1.42	1.38
2	A	1101	2Q6	C26-C27	2.18	1.42	1.39
2	A	1101	2Q6	C40-C39	2.14	1.42	1.38
2	B	1101	2Q6	O4-C30	2.13	1.37	1.34
2	A	1101	2Q6	C6-C7	2.13	1.42	1.39
2	B	1101	2Q6	O1-C18	2.03	1.26	1.22
2	B	1101	2Q6	C35-N4	2.00	1.40	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	2Q6	O4-C30-N3	8.73	120.15	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	2Q6	O4-C30-N3	7.70	119.05	110.91
2	A	1101	2Q6	C31-O4-C30	6.76	123.46	115.63
2	A	1101	2Q6	O4-C30-O3	-6.59	115.02	124.62
2	B	1101	2Q6	C31-O4-C30	6.46	123.11	115.63
2	B	1101	2Q6	O4-C30-O3	-6.39	115.31	124.62
2	A	1101	2Q6	C20-C19-C18	-4.36	104.00	113.00
2	B	1101	2Q6	C22-N1-C11	3.39	121.44	117.52
2	B	1101	2Q6	C33-C32-C28	-3.04	109.84	113.69
2	A	1101	2Q6	C22-N1-C11	2.79	120.74	117.52
2	A	1101	2Q6	C33-C32-C28	-2.54	110.47	113.69
2	B	1101	2Q6	C12-C11-N1	2.33	117.74	113.47
2	A	1101	2Q6	C12-C11-N1	2.14	117.38	113.47

There are no chirality outliers.

All (17) torsion outliers are listed below:

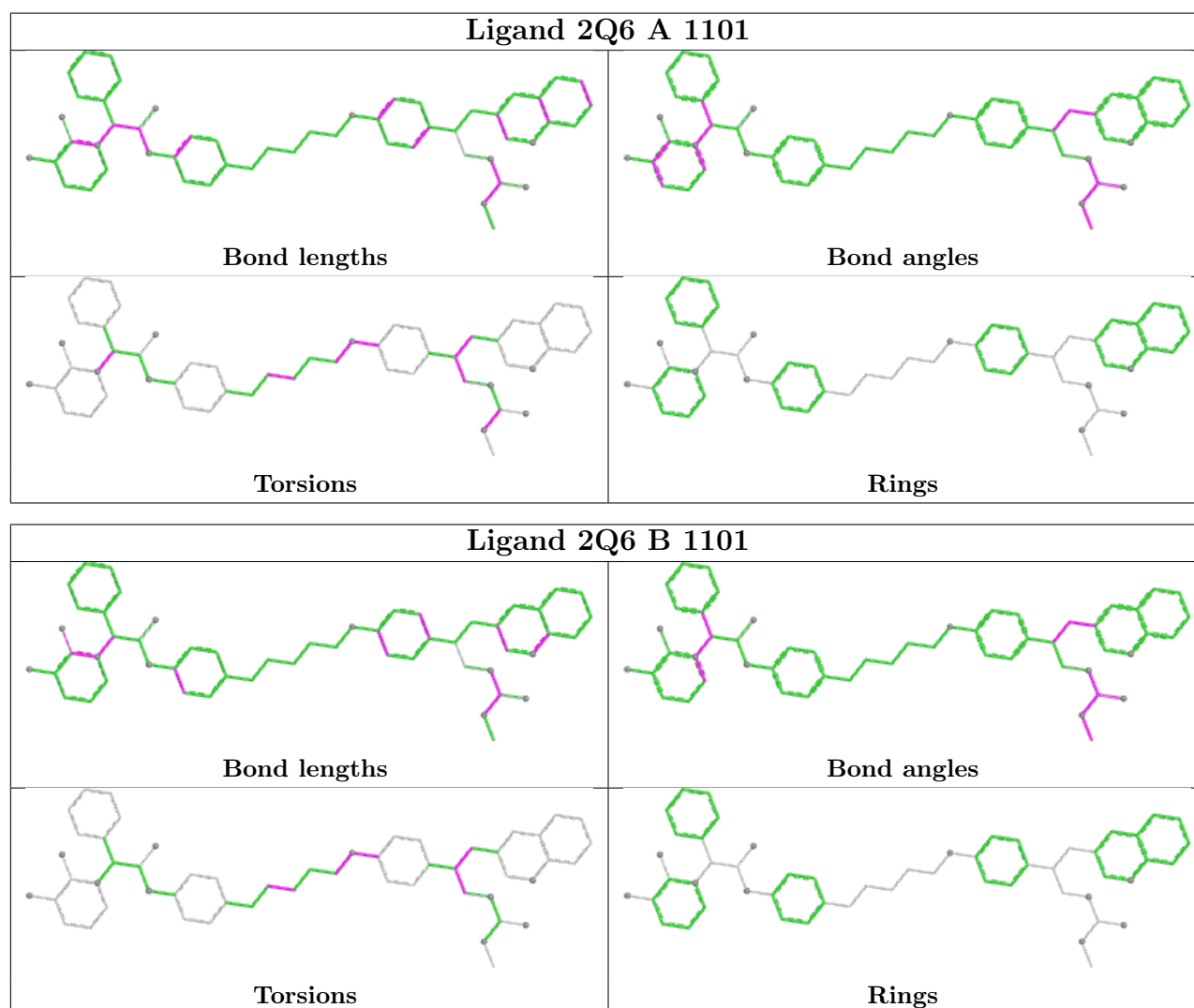
Mol	Chain	Res	Type	Atoms
2	A	1101	2Q6	O3-C30-O4-C31
2	A	1101	2Q6	N3-C30-O4-C31
2	A	1101	2Q6	C32-C28-C29-N3
2	A	1101	2Q6	C27-C28-C29-N3
2	B	1101	2Q6	C32-C28-C29-N3
2	B	1101	2Q6	C27-C28-C29-N3
2	B	1101	2Q6	C25-C24-O2-C23
2	A	1101	2Q6	C-C1-C2-C3
2	B	1101	2Q6	C-C23-O2-C24
2	B	1101	2Q6	C43-C24-O2-C23
2	A	1101	2Q6	C-C23-O2-C24
2	A	1101	2Q6	C43-C24-O2-C23
2	B	1101	2Q6	C-C1-C2-C3
2	A	1101	2Q6	C25-C24-O2-C23
2	A	1101	2Q6	C27-C28-C32-C33
2	B	1101	2Q6	C27-C28-C32-C33
2	A	1101	2Q6	C12-C11-N1-C22

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	2Q6	1	0
2	B	1101	2Q6	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	959/989 (96%)	-0.14	8 (0%) 82 80	25, 44, 70, 118	1 (0%)
1	B	956/989 (96%)	-0.19	8 (0%) 82 80	25, 43, 71, 130	0
All	All	1915/1978 (96%)	-0.17	16 (0%) 82 80	25, 44, 70, 130	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1012	ILE	6.1
1	B	289	PRO	3.9
1	B	290	GLU	3.2
1	B	965	SER	2.9
1	A	965	SER	2.8
1	A	1010	PRO	2.7
1	B	291	HIS	2.7
1	B	1013	ASN	2.6
1	A	857	HIS	2.5
1	A	978	ILE	2.5
1	B	44	ASN	2.3
1	B	175	ASP	2.3
1	A	789	SER	2.3
1	A	1009	LYS	2.2
1	B	980	LEU	2.1
1	A	979	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

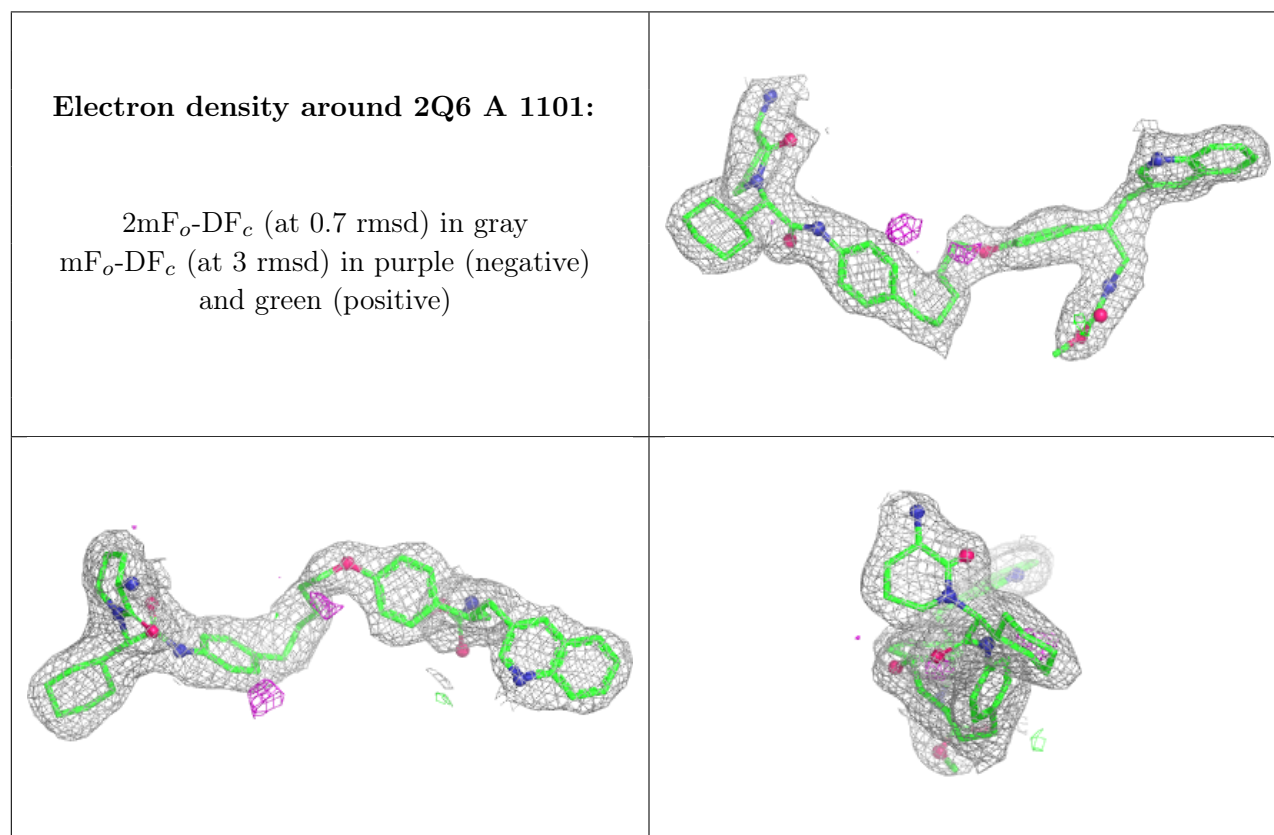
There are no oligosaccharides in this entry.

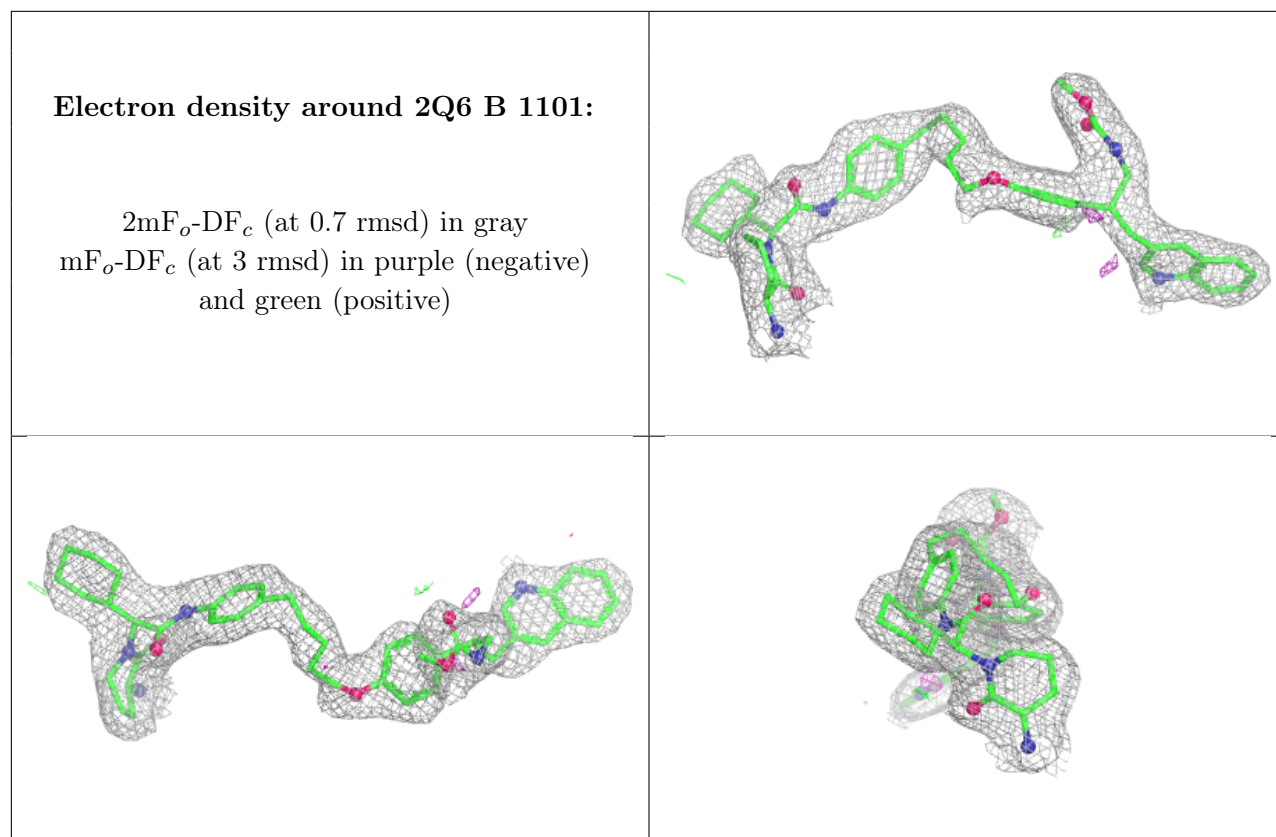
6.4 Ligands [i](#)

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	2Q6	A	1101	54/54	0.91	0.10	30,49,72,75	0
2	2Q6	B	1101	54/54	0.91	0.09	31,40,55,59	0
3	ZN	A	1102	1/1	0.97	0.06	104,104,104,104	0
3	ZN	B	1102	1/1	0.98	0.04	76,76,76,76	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.