



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:57 AM UTC

PDB ID : 7W41 / pdb_00007w41
Title : Crystal Structure of Human Gastrin Releasing Peptide Receptor in complex with the antagonist PD176252
Authors : Peng, S.; Zhan, Y.; Zhang, H.
Deposited on : 2021-11-26
Resolution : 2.95 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

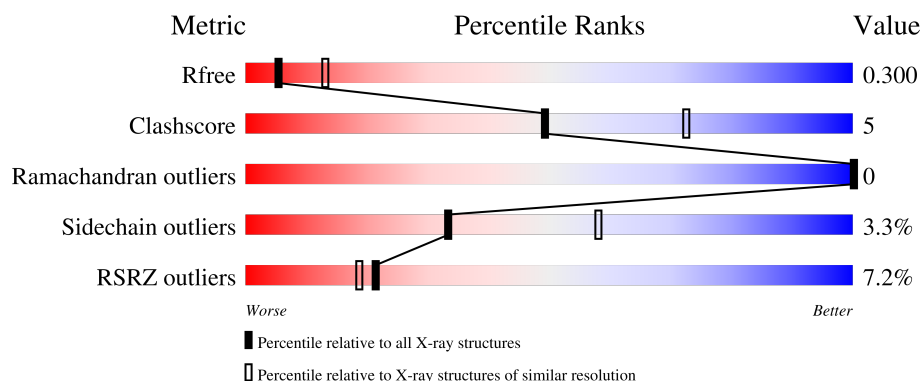
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	484	

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.

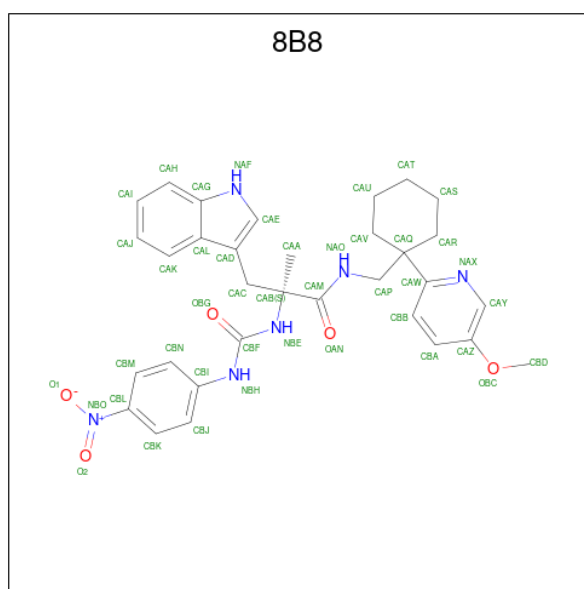
- Molecule 1 is a protein called Gastrin-releasing peptide receptor, G1gA glycogen synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3814	2494	627	670	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	LYS	SER	engineered mutation	UNP P30550
A	157	ALA	ILE	engineered mutation	UNP P30550
A	443	GLU	ARG	engineered mutation	UNP P30550

- Molecule 2 is (2S)-3-(1H-indol-3-yl)-N-[[1-(5-methoxypyridin-2-yl)cyclohexyl]methyl]-2-methyl-2-[(4-nitrophenyl)carbamoylamino]propanamide (CCD ID: 8B8) (formula: C₃₂H₃₆N₆O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	32	6	5		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.10Å 60.02Å 98.49Å 90.00° 113.57° 90.00°	Depositor
Resolution (Å)	27.77 – 2.95 27.77 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.9 (27.77-2.95) 96.9 (27.77-2.95)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.280 , 0.321 (Not available) , 0.300	Depositor DCC
R_{free} test set	1488 reflections (9.71%)	wwPDB-VP
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3857	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% 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: 8B8

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	0.89	0/3900	1.20	6/5276 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	LEU	CA-C-N	5.89	128.10	120.56
1	A	237	LEU	C-N-CA	5.89	128.10	120.56
1	A	506	LEU	CA-C-N	5.26	127.86	120.28
1	A	506	LEU	C-N-CA	5.26	127.86	120.28
1	A	150	ALA	N-CA-C	-5.16	106.25	113.37
1	A	334	VAL	N-CA-C	5.05	115.19	108.11

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	3814	0	3919	39	0
2	A	43	0	0	7	0
All	All	3857	0	3919	42	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (42) 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)
2:A:601:8B8:O2	2:A:601:8B8:NBO	1.68	1.22
1:A:207:PRO:HA	2:A:601:8B8:O1	1.58	1.03
1:A:395:THR:HG21	1:A:432:ARG:HG3	1.75	0.68
1:A:117:PRO:HB2	1:A:175:GLU:HB3	1.75	0.67
1:A:264:LEU:HD21	1:A:349:LEU:HD23	1.78	0.65
1:A:277:MET:HE3	1:A:313:ILE:HD12	1.83	0.59
1:A:51:ILE:HG12	1:A:496:PHE:HE1	1.69	0.56
1:A:149:GLN:C	1:A:151:SER:H	2.15	0.53
1:A:51:ILE:HG12	1:A:496:PHE:CE1	2.45	0.51
1:A:383:ALA:HB1	1:A:388:ARG:HD3	1.94	0.50
1:A:297:GLU:O	1:A:300:SER:OG	2.29	0.50
1:A:274:VAL:HG21	1:A:415:LEU:HD12	1.94	0.49
1:A:230:TYR:HA	1:A:233:ILE:HB	1.95	0.48
1:A:211:SER:HB3	1:A:472:SER:OG	2.14	0.47
1:A:198:PRO:HG3	2:A:601:8B8:CAE	2.44	0.47
1:A:207:PRO:HG3	2:A:601:8B8:O2	2.14	0.47
1:A:418:SER:HA	1:A:422:LEU:HD11	1.96	0.47
2:A:601:8B8:OBG	2:A:601:8B8:CBJ	2.61	0.47
1:A:243:ILE:HG23	1:A:243:ILE:O	2.14	0.47
1:A:40:LEU:O	1:A:44:PRO:HD3	2.14	0.46
1:A:452:VAL:HG11	1:A:509:LEU:HD11	1.97	0.46
1:A:94:ALA:HB3	1:A:95:PRO:HD3	1.97	0.46
1:A:504:PHE:O	1:A:507:TYR:HB3	2.17	0.45
1:A:397:ILE:HG21	1:A:410:ALA:HB1	1.98	0.45
1:A:270:MET:HE1	1:A:335:LYS:HB2	1.99	0.44
1:A:347:ARG:HG3	1:A:375:LEU:HD11	1.99	0.44
1:A:211:SER:HB2	1:A:469:LEU:HA	2.00	0.44
1:A:293:LEU:HD22	1:A:327:LEU:HD12	1.99	0.44
1:A:282:PHE:HA	1:A:289:VAL:HG11	1.98	0.44
1:A:237:LEU:HD22	1:A:444:LYS:HG2	1.99	0.43
1:A:489:ILE:HD12	1:A:489:ILE:HA	1.91	0.43
1:A:355:PHE:CZ	1:A:414:ALA:HB1	2.54	0.43
1:A:121:LEU:HD22	1:A:175:GLU:HG3	2.01	0.43
1:A:328:GLU:HG3	1:A:334:VAL:O	2.19	0.42
1:A:53:ILE:HG23	1:A:504:PHE:CE1	2.55	0.42
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.89	0.42
1:A:399:VAL:HB	1:A:406:GLU:HG2	2.02	0.42
1:A:486:VAL:O	1:A:490:CYS:SG	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLN:C	1:A:151:SER:N	2.78	0.41
2:A:601:8B8:OAN	2:A:601:8B8:CBF	2.65	0.41
1:A:175:GLU:OE1	2:A:601:8B8:NBH	2.53	0.41
1:A:194:ILE:H	1:A:194:ILE:HG13	1.68	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	482/484 (100%)	474 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	418/420 (100%)	404 (97%)	14 (3%)	33	58

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	53	ILE

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Mol	Chain	Res	Type
1	A	148	ILE
1	A	158	CYS
1	A	204	GLU
1	A	206	HIS
1	A	272	GLU
1	A	287	LYS
1	A	290	ASP
1	A	319	GLU
1	A	368	VAL
1	A	393	ASN
1	A	425	PHE
1	A	446	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	409	ASN
1	A	428	ASN
1	A	439	GLN
1	A	498	ASN
1	A	516	GLN

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 ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	8B8	A	601	-	47,47,47	4.56	14 (29%)	62,67,67	1.96	13 (20%)

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	8B8	A	601	-	-	13/36/48/48	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	8B8	O2-NBO	26.62	1.68	1.22
2	A	601	8B8	CAQ-CAW	-7.05	1.42	1.52
2	A	601	8B8	CBL-NBO	-6.18	1.30	1.45
2	A	601	8B8	CBI-NBH	-5.54	1.30	1.41
2	A	601	8B8	CAL-CAD	-5.41	1.35	1.44
2	A	601	8B8	CAC-CAD	5.07	1.59	1.51
2	A	601	8B8	CAL-CAG	-4.98	1.35	1.41
2	A	601	8B8	CAK-CAL	-3.32	1.34	1.39
2	A	601	8B8	CAH-CAG	-2.74	1.35	1.39
2	A	601	8B8	CAY-NAX	2.54	1.39	1.34
2	A	601	8B8	OAN-CAM	2.32	1.26	1.22
2	A	601	8B8	CAG-NAF	-2.13	1.34	1.37
2	A	601	8B8	CAE-NAF	-2.09	1.33	1.37
2	A	601	8B8	CAP-NAO	2.02	1.50	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	8B8	CAP-NAO-CAM	-6.94	114.27	123.21
2	A	601	8B8	CAC-CAB-CAM	5.51	118.42	108.67
2	A	601	8B8	CAM-CAB-NBE	-4.74	101.96	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	8B8	CAY-NAX-CAW	4.04	121.93	117.60
2	A	601	8B8	CAS-CAR-CAQ	-3.90	107.95	113.20
2	A	601	8B8	CAR-CAQ-CAP	-3.30	102.66	109.31
2	A	601	8B8	CBI-NBH-CBF	-3.29	119.89	126.61
2	A	601	8B8	CAR-CAQ-CAW	2.95	117.29	110.69
2	A	601	8B8	CBB-CAW-NAX	-2.71	119.06	122.33
2	A	601	8B8	CAJ-CAI-CAH	-2.66	116.96	120.24
2	A	601	8B8	CBN-CBI-CBJ	2.27	122.05	119.04
2	A	601	8B8	CAD-CAE-NAF	-2.03	108.08	110.31
2	A	601	8B8	CAL-CAD-CAE	2.01	108.22	106.16

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	8B8	CBK-CBL-NBO-O2
2	A	601	8B8	CBM-CBL-NBO-O2
2	A	601	8B8	CAC-CAB-CAM-OAN
2	A	601	8B8	CAP-CAQ-CAW-NAX
2	A	601	8B8	CAR-CAQ-CAW-NAX
2	A	601	8B8	CAV-CAQ-CAW-NAX
2	A	601	8B8	NBE-CAB-CAM-OAN
2	A	601	8B8	CAC-CAB-CAM-NAO
2	A	601	8B8	CAR-CAQ-CAW-CBB
2	A	601	8B8	NAO-CAP-CAQ-CAW
2	A	601	8B8	NBE-CAB-CAM-NAO
2	A	601	8B8	CAP-CAQ-CAW-CBB
2	A	601	8B8	CAV-CAQ-CAW-CBB

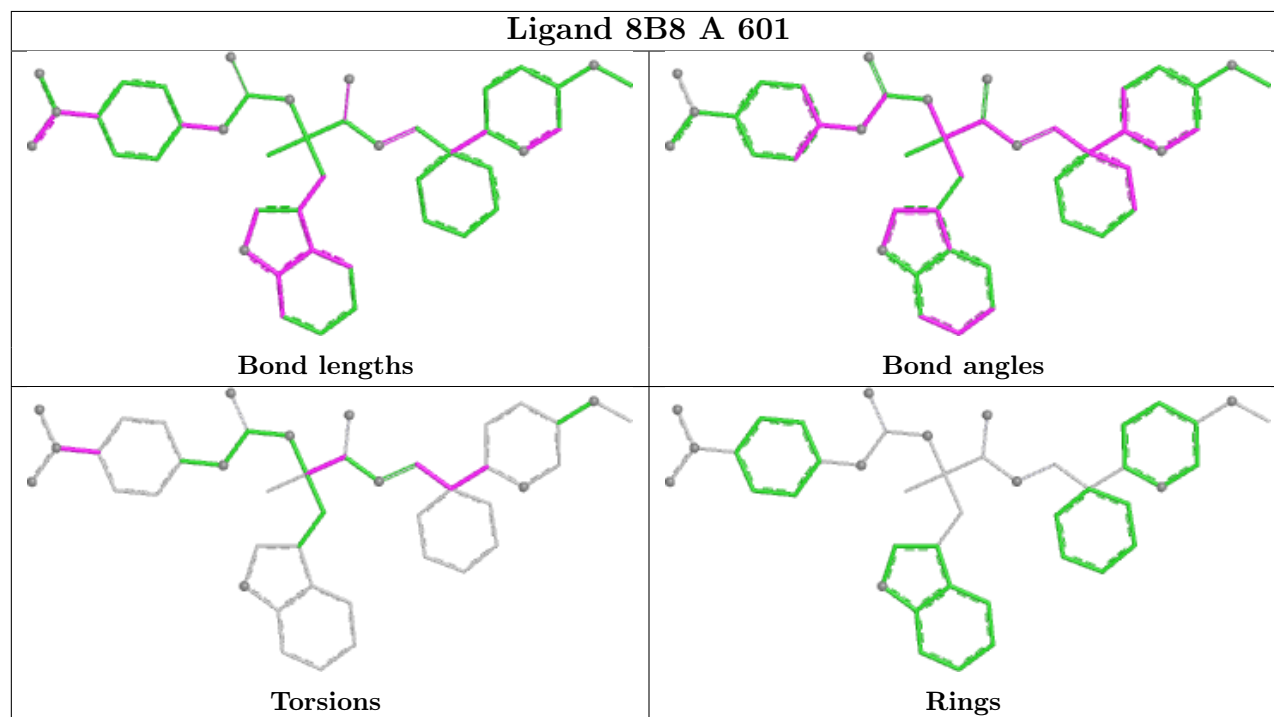
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	8B8	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	484/484 (100%)	0.60	35 (7%)	21 19	53, 83, 125, 158	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	ARG	5.9
1	A	38	GLY	5.5
1	A	471	ARG	4.8
1	A	150	ALA	4.8
1	A	151	SER	4.7
1	A	475	TYR	3.9
1	A	201	HIS	3.7
1	A	104	ASP	3.6
1	A	315	LYS	3.6
1	A	472	SER	3.4
1	A	146	MET	3.3
1	A	316	GLY	3.3
1	A	283	ASP	3.2
1	A	147	ASP	3.2
1	A	41	TYR	2.9
1	A	202	SER	2.9
1	A	188	SER	2.9
1	A	67	THR	2.9
1	A	476	SER	2.8
1	A	285	GLY	2.8
1	A	187	GLU	2.7
1	A	39	ILE	2.6
1	A	521	LEU	2.6
1	A	271	ASP	2.4
1	A	389	ASP	2.4
1	A	199	TYR	2.3
1	A	249	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	65	PHE	2.2
1	A	40	LEU	2.2
1	A	218	PHE	2.2
1	A	403	ASP	2.2
1	A	179	SER	2.2
1	A	513	PHE	2.1
1	A	50	ILE	2.1
1	A	144	ARG	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](#)

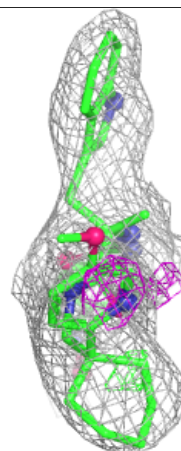
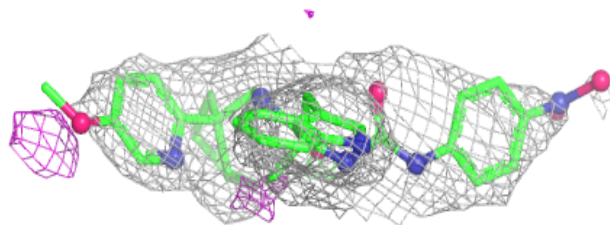
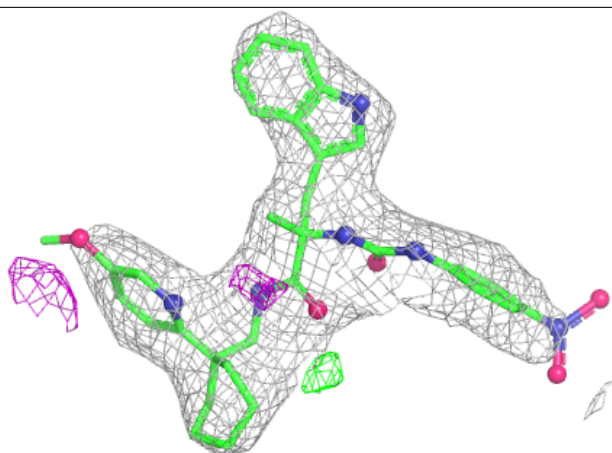
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	8B8	A	601	43/43	0.86	0.17	65,87,111,124	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 8B8 A 601:

$2mF_o-DF_c$ (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.