



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 07:31 AM EST

PDB ID : 2OHN  
Title : X-ray crystal structure of beta secretase complexed with 4-(4-fluorobenzyl)pi  
peridine  
Authors : Patel, S.  
Deposited on : 2007-01-10  
Resolution : 2.15 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

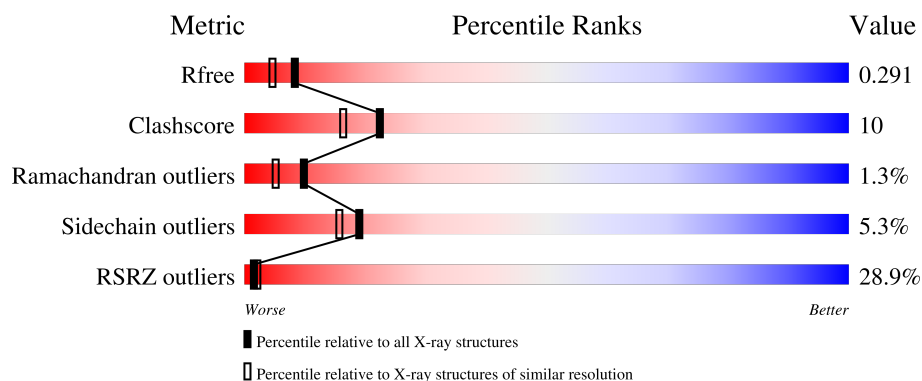
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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  $\geq 3$ , 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	402	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3240 atoms, of which 17 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	377	2966	1898	493	561	14	0	0	0

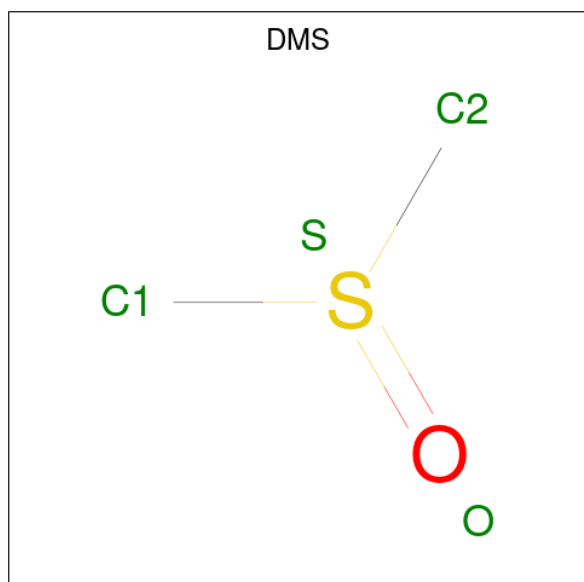
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LYS	ARG	engineered mutation	UNP P56817
A	-4	LYS	ARG	engineered mutation	UNP P56817

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

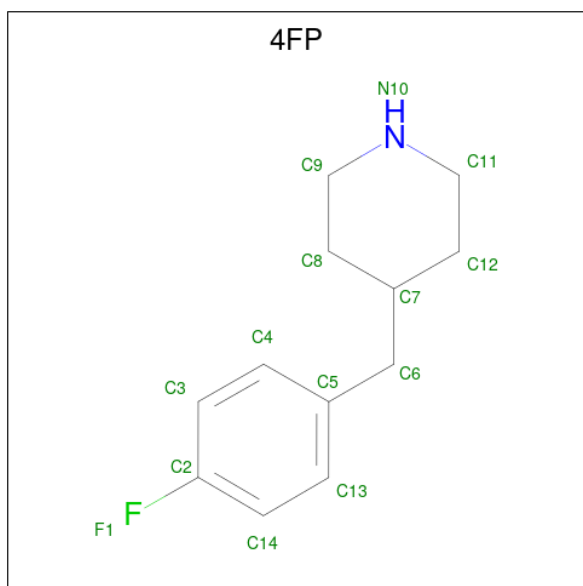
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	I	0	0
			3	3		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is 4-(4-FLUOROBENZYL)PIPERIDINE (three-letter code: 4FP) (formula: C<sub>12</sub>H<sub>16</sub>FN).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	H	N	0	0
			31	12	1	17	1		

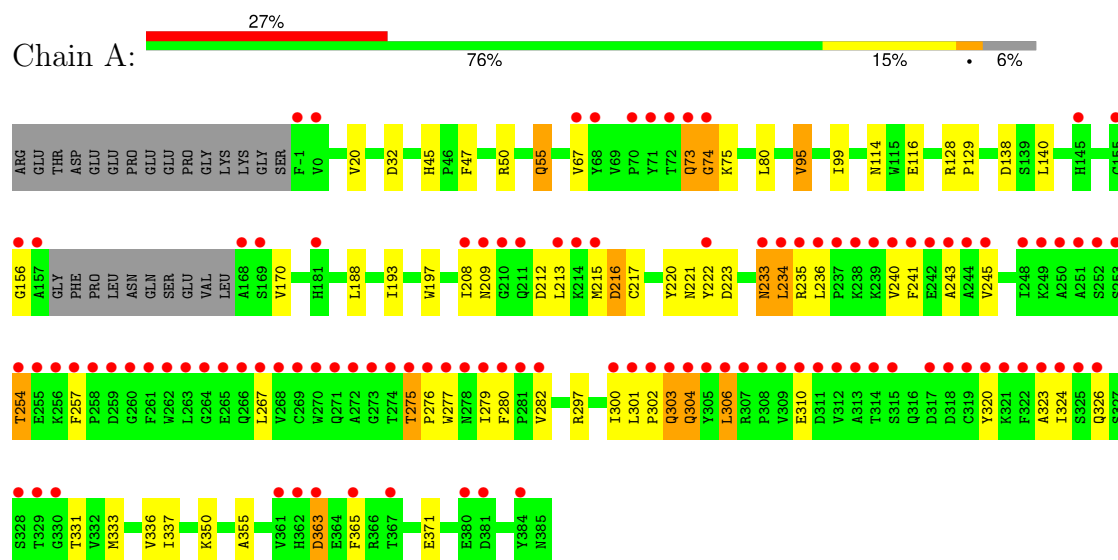
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	236	Total	O	0	0
			236	236		

### 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: Beta-secretase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.39Å 102.39Å 170.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.79 – 2.15 47.79 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.79-2.15) 99.4 (47.79-2.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019g	Depositor
R, $R_{free}$	0.228 , 0.285 0.236 , 0.291	Depositor DCC
$R_{free}$ test set	1487 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 4FP, IOD, DMS

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	0.58	0/3041	0.70	0/4132

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	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	ASN	Peptide
1	A	74	GLY	Peptide

### 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	2966	0	2878	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	0	0
3	A	4	0	6	0	0
4	A	14	17	16	1	0
5	A	236	0	0	5	0
All	All	3223	17	2900	61	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 10.

All (61) 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:304:GLN:HE21	1:A:304:GLN:N	1.69	0.90
1:A:300:ILE:O	1:A:301:LEU:HD23	1.75	0.85
1:A:320:TYR:HB3	5:A:622:HOH:O	1.85	0.75
1:A:241:PHE:CD2	1:A:326:GLN:HG2	2.24	0.72
1:A:209:ASN:HA	1:A:282:VAL:HG22	1.74	0.70
1:A:212:ASP:OD2	5:A:608:HOH:O	2.10	0.69
1:A:221:ASN:O	5:A:606:HOH:O	2.12	0.66
1:A:215:MET:HE1	1:A:243:ALA:HB3	1.79	0.64
1:A:254:THR:HG21	1:A:279:ILE:HD12	1.82	0.62
1:A:300:ILE:HG21	1:A:337:ILE:HD13	1.81	0.62
1:A:208:ILE:HD12	1:A:213:LEU:HD11	1.82	0.62
1:A:241:PHE:CZ	1:A:245:VAL:HG21	2.35	0.61
1:A:156:GLY:HA2	1:A:170:VAL:HG12	1.83	0.60
1:A:302:PRO:O	1:A:306:LEU:N	2.29	0.60
1:A:254:THR:CB	1:A:279:ILE:HD12	2.32	0.59
1:A:67:VAL:HG12	1:A:129:PRO:HD3	1.86	0.58
1:A:302:PRO:O	1:A:306:LEU:HB2	2.04	0.57
1:A:45:HIS:HD2	1:A:47:PHE:H	1.52	0.56
1:A:20:VAL:HG11	1:A:99:ILE:HD13	1.87	0.56
1:A:234:LEU:O	1:A:324:ILE:HA	2.05	0.55
1:A:323:ALA:HB1	1:A:336:VAL:HG21	1.87	0.55
1:A:235:ARG:O	1:A:331:THR:HA	2.07	0.55
1:A:156:GLY:HA2	1:A:170:VAL:CG1	2.38	0.54
1:A:156:GLY:HA2	1:A:170:VAL:CB	2.38	0.54
1:A:236:LEU:O	1:A:326:GLN:HA	2.08	0.53
1:A:254:THR:OG1	1:A:279:ILE:HG23	2.08	0.53
1:A:275:THR:HG22	1:A:276:PRO:HD2	1.90	0.53
1:A:156:GLY:HA2	1:A:170:VAL:HB	1.91	0.53
1:A:215:MET:CE	1:A:243:ALA:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:TYR:HA	1:A:240:VAL:HG21	1.92	0.52
1:A:279:ILE:HG22	1:A:279:ILE:O	2.10	0.52
1:A:254:THR:HG21	1:A:279:ILE:CD1	2.40	0.51
1:A:363:ASP:OD2	1:A:365:PHE:N	2.40	0.48
1:A:254:THR:CG2	1:A:279:ILE:HD12	2.42	0.48
1:A:304:GLN:HE21	1:A:304:GLN:CA	2.26	0.48
1:A:32:ASP:OD2	4:A:405:4FP:H81	2.14	0.47
1:A:50:ARG:O	1:A:116:GLU:HG2	2.15	0.46
1:A:300:ILE:HD13	1:A:337:ILE:HD13	1.99	0.45
1:A:280:PHE:HB2	1:A:302:PRO:HG2	1.98	0.45
1:A:306:LEU:HA	5:A:622:HOH:O	2.16	0.45
1:A:241:PHE:CE1	1:A:245:VAL:CG2	3.00	0.44
1:A:20:VAL:HG11	1:A:99:ILE:CD1	2.47	0.44
1:A:215:MET:O	1:A:216:ASP:C	2.56	0.44
1:A:67:VAL:CG1	1:A:129:PRO:HD3	2.48	0.43
1:A:193:ILE:HD12	1:A:350:LYS:HA	2.00	0.43
1:A:50:ARG:HH22	1:A:114:ASN:ND2	2.17	0.42
1:A:55:GLN:NE2	5:A:549:HOH:O	2.46	0.42
1:A:95:VAL:HG11	1:A:140:LEU:HD13	2.01	0.42
1:A:67:VAL:CG1	1:A:80:LEU:HD11	2.50	0.42
1:A:301:LEU:HB2	1:A:303:GLN:HG2	2.01	0.42
1:A:45:HIS:CD2	1:A:47:PHE:H	2.34	0.42
1:A:241:PHE:CE1	1:A:245:VAL:HG23	2.54	0.42
1:A:217:CYS:HA	1:A:220:TYR:CD1	2.55	0.42
1:A:188:LEU:HD23	1:A:355:ALA:HB2	2.02	0.41
1:A:300:ILE:HD13	1:A:337:ILE:CD1	2.50	0.41
1:A:297:ARG:NH2	1:A:371:GLU:OE2	2.49	0.41
1:A:304:GLN:C	1:A:336:VAL:HG13	2.41	0.41
1:A:300:ILE:HG13	1:A:301:LEU:N	2.36	0.41
1:A:333:MET:HE2	1:A:337:ILE:HG21	2.03	0.41
1:A:55:GLN:HE21	1:A:55:GLN:H	1.67	0.41
1:A:222:TYR:HA	1:A:223:ASP:HA	1.79	0.41

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	373/402 (93%)	351 (94%)	17 (5%)	5 (1%)	10 5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	310	GLU
1	A	363	ASP
1	A	216	ASP
1	A	74	GLY

### 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	321/343 (94%)	304 (95%)	17 (5%)	19 16

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	73	GLN
1	A	75	LYS
1	A	95	VAL
1	A	128	ARG
1	A	138	ASP
1	A	197	TRP
1	A	233	ASN
1	A	234	LEU
1	A	254	THR
1	A	257	PHE
1	A	267	LEU

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Mol	Chain	Res	Type
1	A	275	THR
1	A	277	TRP
1	A	303	GLN
1	A	304	GLN
1	A	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	45	HIS
1	A	55	GLN
1	A	114	ASN
1	A	211	GLN
1	A	266	GLN
1	A	271	GLN
1	A	278	ASN
1	A	304	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 5 ligands modelled in this entry, 3 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	$\# Z  > 2$
4	4FP	A	405	-	15,15,15	0.52	0	19,19,19	0.88	1 (5%)
3	DMS	A	404	-	3,3,3	2.85	1 (33%)	3,3,3	0.76	0

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
4	4FP	A	405	-	-	1/4/12/12	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	DMS	O-S	4.75	1.81	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	4FP	C14-C2-C3	-2.19	119.93	122.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	4FP	C5-C6-C7-C12

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	4FP	1	0

## 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	377/402 (93%)	1.22	109 (28%) <b>1</b> <b>2</b>	20, 37, 89, 117	2 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	TRP	8.3
1	A	305	TYR	7.7
1	A	276	PRO	7.5
1	A	280	PHE	7.4
1	A	313	ALA	7.1
1	A	306	LEU	6.8
1	A	314	THR	6.4
1	A	272	ALA	6.3
1	A	245	VAL	6.2
1	A	258	PRO	5.7
1	A	257	PHE	5.4
1	A	74	GLY	5.4
1	A	309	VAL	5.3
1	A	72	THR	5.3
1	A	365	PHE	5.3
1	A	312	VAL	5.3
1	A	157	ALA	5.2
1	A	267	LEU	5.2
1	A	322	PHE	5.1
1	A	282	VAL	5.1
1	A	262	TRP	5.0
1	A	318	ASP	5.0
1	A	279	ILE	4.9
1	A	308	PRO	4.8
1	A	281	PRO	4.6
1	A	268	VAL	4.6
1	A	320	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	319	CYS	4.5
1	A	275	THR	4.5
1	A	254	THR	4.5
1	A	250	ALA	4.4
1	A	270	TRP	4.4
1	A	367	THR	4.4
1	A	244	ALA	4.3
1	A	71	TYR	4.3
1	A	251	ALA	4.2
1	A	260	GLY	4.2
1	A	261	PHE	4.2
1	A	323	ALA	4.1
1	A	384	TYR	4.1
1	A	263	LEU	4.1
1	A	73	GLN	4.0
1	A	68	TYR	3.9
1	A	274	THR	3.8
1	A	273	GLY	3.8
1	A	310	GLU	3.8
1	A	302	PRO	3.8
1	A	248	ILE	3.8
1	A	301	LEU	3.8
1	A	215	MET	3.7
1	A	307	ARG	3.6
1	A	256	LYS	3.6
1	A	315	SER	3.5
1	A	266	GLN	3.4
1	A	209	ASN	3.4
1	A	278	ASN	3.4
1	A	324	ILE	3.4
1	A	328	SER	3.2
1	A	0	VAL	3.1
1	A	210	GLY	3.1
1	A	241	PHE	3.0
1	A	325	SER	3.0
1	A	242	GLU	3.0
1	A	259	ASP	3.0
1	A	311	ASP	3.0
1	A	236	LEU	3.0
1	A	208	ILE	3.0
1	A	240	VAL	2.9
1	A	213	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	238	LYS	2.8
1	A	233	ASN	2.8
1	A	156	GLY	2.8
1	A	326	GLN	2.8
1	A	253	SER	2.8
1	A	239	LYS	2.7
1	A	321	LYS	2.7
1	A	363	ASP	2.7
1	A	271	GLN	2.7
1	A	304	GLN	2.7
1	A	249	LYS	2.7
1	A	252	SER	2.7
1	A	169	SER	2.6
1	A	70	PRO	2.6
1	A	317	ASP	2.6
1	A	237	PRO	2.6
1	A	300	ILE	2.5
1	A	362	HIS	2.5
1	A	234	LEU	2.5
1	A	361	VAL	2.5
1	A	381	ASP	2.4
1	A	303	GLN	2.4
1	A	255	GLU	2.4
1	A	329	THR	2.4
1	A	155	CYS	2.3
1	A	269	CYS	2.3
1	A	235	ARG	2.3
1	A	181	HIS	2.3
1	A	168	ALA	2.3
1	A	264	GLY	2.3
1	A	-1	PHE	2.3
1	A	330	GLY	2.2
1	A	211	GLN	2.2
1	A	243	ALA	2.2
1	A	67	VAL	2.2
1	A	380	GLU	2.1
1	A	265	GLU	2.1
1	A	145	HIS	2.1
1	A	222	TYR	2.1
1	A	214	LYS	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 monosaccharides 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, 95<sup>th</sup> 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
4	4FP	A	405	14/14	0.82	0.14	38,48,58,61	0
3	DMS	A	404	4/4	0.90	0.20	63,65,66,69	0
2	IOD	A	403	1/1	0.95	0.16	33,33,33,33	1
2	IOD	A	402	1/1	0.96	0.39	59,59,59,59	1
2	IOD	A	401	1/1	1.00	0.05	25,25,25,25	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.