



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:01 PM GMT

PDB ID : 4K9H  
Title : Bace-1 inhibitor complex  
Authors : Jordan, S.R.  
Deposited on : 2013-04-19  
Resolution : 2.29 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

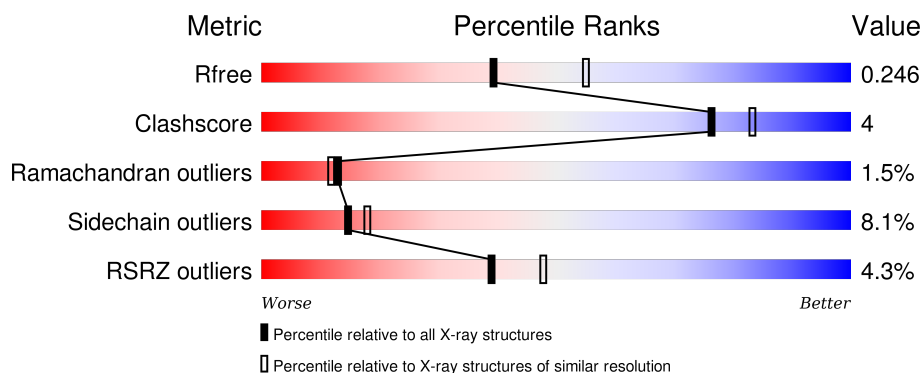
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	388	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>5%</div> </div> </div>
1	B	388	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>5%</div> </div> </div>
1	C	388	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

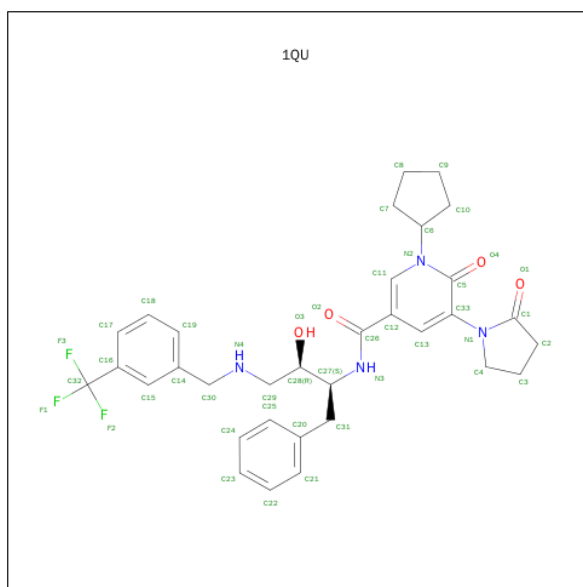
There are 3 unique types of molecules in this entry. The entry contains 8879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2915	1869	485	547	14			
1	B	369	Total	C	N	O	S	0	0	0
			2909	1866	484	545	14			
1	C	370	Total	C	N	O	S	0	0	0
			2915	1869	485	547	14			

- Molecule 2 is 1-CYCLOPENTYL-N-[(2S,3R)-3-HYDROXY-1-PHENYL-4-{[3-(TRIFLUOROMETHYL)BENZYL]AMINO}BUTAN-2-YL]-6-OXO-5-(2-OXOPYRROLIDIN-1-YL)-1,6-DIHYDROPYRIDINE-3-CARBOXAMIDE (three-letter code: 1QU) (formula: C<sub>33</sub>H<sub>37</sub>F<sub>3</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			44	33	3	4	4		
2	B	1	Total	C	F	N	O	0	0
			44	33	3	4	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	0	0
			44	33	3	4	4		

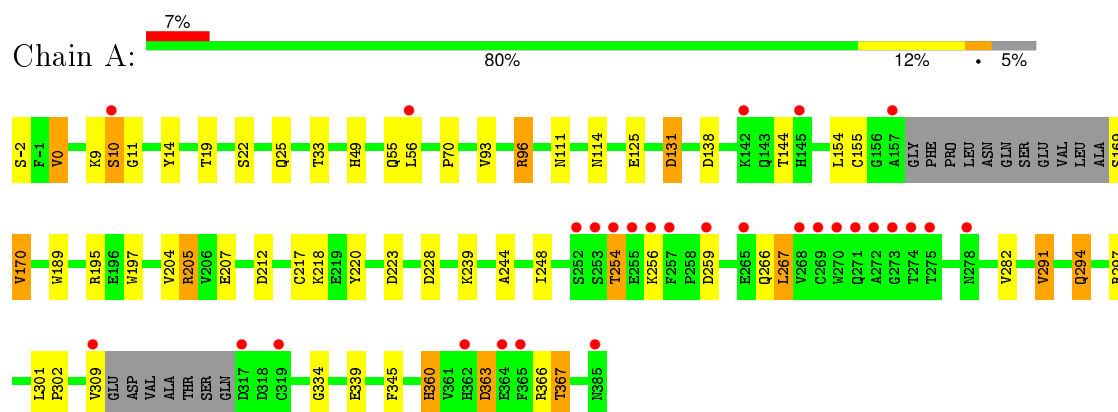
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	3	Total	O	0	0
			3	3		
3	C	3	Total	O	0	0
			3	3		

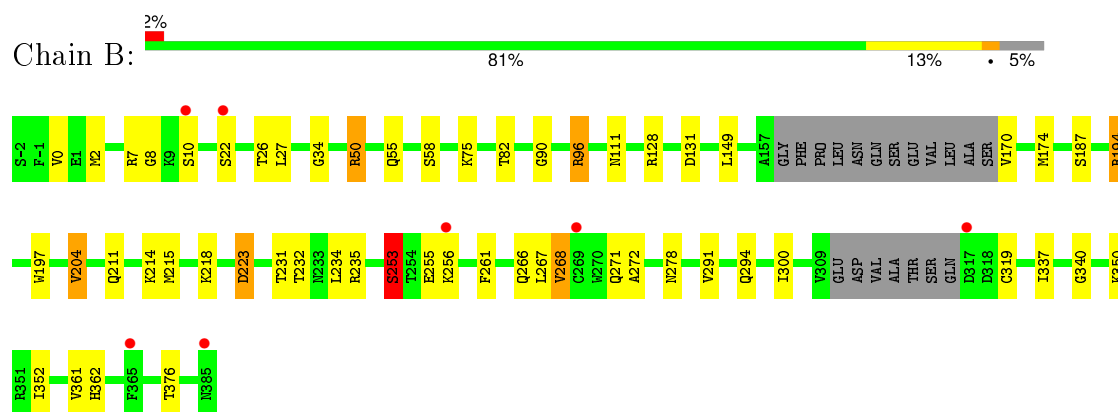
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

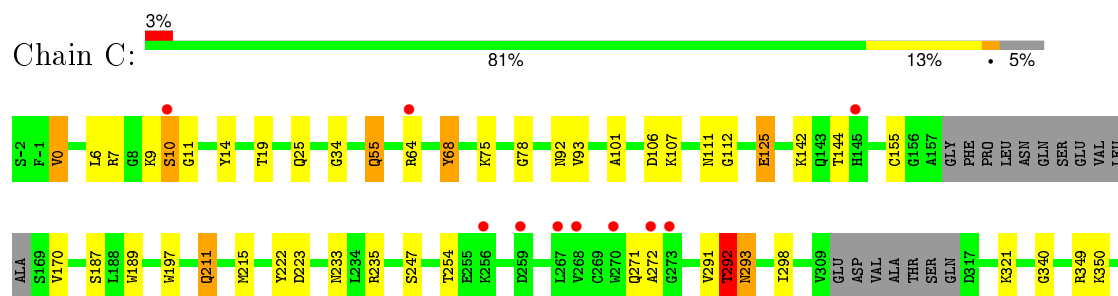
#### • Molecule 1: Beta-secretase 1

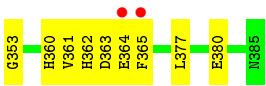


#### • Molecule 1: Beta-secretase 1



#### • Molecule 1: Beta-secretase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.54Å 103.30Å 100.86Å 90.00° 104.01° 90.00°	Depositor
Resolution (Å)	44.00 – 2.29 44.22 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.4 (44.00-2.29) 94.4 (44.22-2.29)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.199 , 0.248 0.204 , 0.246	Depositor DCC
$R_{free}$ test set	3702 reflections (5.62%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 69365 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 1QU

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	0.88	0/2989	0.96	6/4060 (0.1%)
1	B	0.96	0/2983	0.99	8/4052 (0.2%)
1	C	0.91	1/2989 (0.0%)	0.95	4/4060 (0.1%)
All	All	0.92	1/8961 (0.0%)	0.97	18/12172 (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
1	C	0	3
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	TYR	CB-CG	-5.70	1.43	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	A	96	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	C	235	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	C	235	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	0	VAL	CB-CA-C	-5.92	100.16	111.40
1	A	138	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	174	MET	CG-SD-CE	-5.75	91.01	100.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	C	292	THR	N-CA-CB	5.60	120.94	110.30
1	C	0	VAL	CB-CA-C	-5.59	100.79	111.40
1	B	50	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	363	ASP	N-CA-C	-5.32	96.64	111.00
1	B	7	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	223	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	B	7	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	194	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	297	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	96	ARG	CG-CD-NE	-5.05	101.20	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	340	GLY	Peptide
1	C	222	TYR	Peptide
1	C	292	THR	Peptide
1	C	340	GLY	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	2915	0	2833	23	0
1	B	2909	0	2828	17	0
1	C	2915	0	2833	27	0
2	A	44	0	37	0	0
2	B	44	0	36	3	0
2	C	44	0	36	2	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
All	All	8879	0	8603	66	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 4.

All (66) 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:C:55:GLN:H	1:C:55:GLN:HE21	1.26	0.79
1:C:10:SER:OG	1:C:11:GLY:N	2.20	0.74
1:A:10:SER:OG	1:A:11:GLY:N	2.25	0.70
1:C:9:LYS:O	1:C:10:SER:HB3	1.91	0.70
1:C:363:ASP:O	1:C:365:PHE:N	2.26	0.68
1:A:205:ARG:NH2	1:A:207:GLU:OE2	2.31	0.64
1:C:9:LYS:O	1:C:10:SER:CB	2.46	0.64
1:C:55:GLN:NE2	1:C:55:GLN:H	1.97	0.63
1:B:271:GLN:OE1	1:B:271:GLN:N	2.31	0.62
1:A:266:GLN:O	1:A:267:LEU:HB2	2.00	0.61
1:A:205:ARG:NH1	1:A:212:ASP:OD2	2.35	0.59
1:A:155:CYS:O	1:A:170:VAL:HG22	2.05	0.56
1:C:292:THR:O	1:C:293:ASN:CB	2.51	0.56
1:A:291:VAL:HG12	1:A:294:GLN:HB3	1.87	0.55
1:B:204:VAL:HG13	1:B:376:THR:HG21	1.89	0.55
1:C:125:GLU:HG3	1:C:125:GLU:O	2.09	0.53
1:A:93:VAL:HG21	1:A:144:THR:CG2	2.39	0.52
1:A:33:THR:HG21	1:A:345:PHE:CZ	2.44	0.52
1:C:291:VAL:O	1:C:292:THR:HG23	2.10	0.52
1:A:154:LEU:O	1:A:339:GLU:HA	2.10	0.51
1:A:205:ARG:CZ	1:A:212:ASP:OD2	2.59	0.51
1:C:155:CYS:O	1:C:170:VAL:HG13	2.11	0.50
1:B:261:PHE:CE1	1:B:268:VAL:HG23	2.49	0.48
1:A:93:VAL:HG21	1:A:144:THR:HG21	1.95	0.48
1:A:244:ALA:O	1:A:248:ILE:HG13	2.13	0.47
1:B:271:GLN:O	1:B:272:ALA:C	2.53	0.47
1:C:233:ASN:HB2	2:C:401:1QU:H3	1.96	0.47
1:A:301:LEU:HB3	1:A:302:PRO:HD2	1.97	0.46
1:A:217:CYS:HA	1:A:220:TYR:CD2	2.50	0.46
1:A:291:VAL:HG12	1:A:294:GLN:CB	2.45	0.46
1:B:34:GLY:O	2:B:401:1QU:H35	2.16	0.46
1:B:149:LEU:N	1:B:149:LEU:HD23	2.31	0.46
1:A:56:LEU:HD12	1:A:56:LEU:O	2.16	0.46
1:B:234:LEU:HB2	1:B:337:ILE:HD11	1.98	0.46
1:C:292:THR:O	1:C:293:ASN:HB3	2.16	0.45
1:C:78:GLY:HA3	1:C:101:ALA:O	2.17	0.45
1:C:189:TRP:O	1:C:353:GLY:HA2	2.17	0.45
1:C:349:ARG:O	1:C:350:LYS:HB2	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:O	1:C:7:ARG:NH1	2.50	0.44
1:A:204:VAL:O	1:A:205:ARG:HG2	2.18	0.44
1:A:189:TRP:CZ3	1:B:291:VAL:HG13	2.53	0.44
1:B:350:LYS:HB3	1:B:350:LYS:HE3	1.75	0.43
1:A:19:THR:HA	1:A:25:GLN:O	2.18	0.43
1:C:106:ASP:OD1	1:C:107:LYS:HG3	2.19	0.43
1:C:14:TYR:CE2	1:C:170:VAL:CG1	3.01	0.43
1:B:231:THR:HG23	2:B:401:1QU:H5	2.00	0.43
1:B:232:THR:OG1	2:B:401:1QU:H10	2.19	0.43
1:C:93:VAL:HG21	1:C:144:THR:HG21	2.01	0.42
1:A:363:ASP:HB3	1:A:366:ARG:H	1.83	0.42
1:C:9:LYS:HE2	1:C:112:GLY:O	2.19	0.42
1:B:82:THR:HB	1:B:96:ARG:HD3	2.01	0.42
1:A:14:TYR:CE2	1:A:170:VAL:HG13	2.54	0.42
1:C:9:LYS:CE	1:C:112:GLY:O	2.68	0.42
1:C:19:THR:HA	1:C:25:GLN:O	2.20	0.42
1:B:253:SER:C	1:B:255:GLU:H	2.23	0.41
1:A:360:HIS:CE1	1:A:367:THR:HG22	2.55	0.41
1:C:93:VAL:HG21	1:C:144:THR:CG2	2.50	0.41
1:C:14:TYR:CE2	1:C:170:VAL:HG12	2.56	0.41
1:B:8:GLY:C	1:B:170:VAL:HG12	2.41	0.41
1:C:34:GLY:O	2:C:401:1QU:H35	2.20	0.41
1:C:298:ILE:HG21	1:C:298:ILE:HD13	1.77	0.41
1:C:211:GLN:HB2	1:C:211:GLN:HE21	1.71	0.41
1:A:228:ASP:O	1:A:334:GLY:HA2	2.21	0.40
1:B:268:VAL:O	1:B:319:CYS:HA	2.21	0.40
1:B:2:MET:HG2	1:B:90:GLY:HA2	2.04	0.40
1:B:26:THR:C	1:B:27:LEU:HG	2.42	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	364/388 (94%)	342 (94%)	15 (4%)	7 (2%)	10	8
1	B	363/388 (94%)	349 (96%)	11 (3%)	3 (1%)	24	27
1	C	364/388 (94%)	343 (94%)	15 (4%)	6 (2%)	12	11
All	All	1091/1164 (94%)	1034 (95%)	41 (4%)	16 (2%)	13	12

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	LEU
1	B	10	SER
1	B	223	ASP
1	C	10	SER
1	C	272	ALA
1	C	364	GLU
1	A	254	THR
1	A	10	SER
1	A	131	ASP
1	A	223	ASP
1	C	223	ASP
1	A	125	GLU
1	B	253	SER
1	A	70	PRO
1	C	254	THR
1	C	292	THR

### 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	316/331 (96%)	290 (92%)	26 (8%)	14	17
1	B	315/331 (95%)	287 (91%)	28 (9%)	12	14
1	C	316/331 (96%)	293 (93%)	23 (7%)	17	22
All	All	947/993 (95%)	870 (92%)	77 (8%)	15	18

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	0	VAL
1	A	9	LYS
1	A	22	SER
1	A	49	HIS
1	A	55	GLN
1	A	96	ARG
1	A	111	ASN
1	A	114	ASN
1	A	131	ASP
1	A	169	SER
1	A	170	VAL
1	A	195	ARG
1	A	197	TRP
1	A	205	ARG
1	A	218	LYS
1	A	239	LYS
1	A	254	THR
1	A	256	LYS
1	A	259	ASP
1	A	282	VAL
1	A	291	VAL
1	A	294	GLN
1	A	309	VAL
1	A	360	HIS
1	A	367	THR
1	B	0	VAL
1	B	22	SER
1	B	50	ARG
1	B	55	GLN
1	B	58	SER
1	B	75	LYS
1	B	96	ARG
1	B	111	ASN
1	B	131	ASP
1	B	187	SER
1	B	194	ARG
1	B	197	TRP
1	B	204	VAL
1	B	211	GLN
1	B	214	LYS
1	B	215	MET
1	B	218	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	253	SER
1	B	256	LYS
1	B	266	GLN
1	B	267	LEU
1	B	268	VAL
1	B	278	ASN
1	B	294	GLN
1	B	300	ILE
1	B	352	ILE
1	B	361	VAL
1	B	362	HIS
1	C	0	VAL
1	C	55	GLN
1	C	64	ARG
1	C	68	TYR
1	C	75	LYS
1	C	92	ASN
1	C	111	ASN
1	C	125	GLU
1	C	142	LYS
1	C	187	SER
1	C	197	TRP
1	C	211	GLN
1	C	215	MET
1	C	247	SER
1	C	271	GLN
1	C	292	THR
1	C	293	ASN
1	C	321	LYS
1	C	360	HIS
1	C	361	VAL
1	C	362	HIS
1	C	377	LEU
1	C	380	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	271	GLN
1	A	304	GLN
1	A	360	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	28	ASN
1	B	111	ASN
1	B	278	ASN
1	C	28	ASN
1	C	53	GLN
1	C	55	GLN
1	C	98	ASN
1	C	111	ASN
1	C	271	GLN
1	C	326	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	1QU	A	401	-	46,48,48	1.83	7 (15%)	57,68,68	1.42	6 (10%)
2	1QU	B	401	-	46,48,48	1.97	7 (15%)	57,68,68	2.56	14 (24%)
2	1QU	C	401	-	46,48,48	1.54	6 (13%)	57,68,68	2.40	12 (21%)

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	1QU	A	401	-	-	0/32/53/53	0/5/5/5
2	1QU	B	401	-	-	0/32/53/53	0/5/5/5
2	1QU	C	401	-	-	0/32/53/53	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	1QU	C33-N1	-9.17	1.31	1.44
2	B	401	1QU	C33-N1	-8.53	1.32	1.44
2	C	401	1QU	C33-N1	-6.49	1.35	1.44
2	B	401	1QU	C6-N2	-4.16	1.42	1.49
2	B	401	1QU	C11-C12	-3.46	1.33	1.39
2	A	401	1QU	C5-N2	-2.47	1.34	1.38
2	B	401	1QU	C7-C6	-2.25	1.49	1.52
2	C	401	1QU	C5-N2	-2.16	1.35	1.38
2	A	401	1QU	C28-C27	-2.16	1.50	1.54
2	B	401	1QU	C1-N1	-2.13	1.33	1.36
2	C	401	1QU	C12-C26	2.09	1.54	1.50
2	A	401	1QU	C7-C6	2.46	1.56	1.52
2	B	401	1QU	O3-C28	2.47	1.48	1.43
2	C	401	1QU	C31-C27	2.49	1.59	1.53
2	C	401	1QU	C29-N4	2.53	1.51	1.47
2	A	401	1QU	C30-C14	2.61	1.57	1.51
2	A	401	1QU	C12-C26	2.63	1.55	1.50
2	C	401	1QU	C11-N2	4.10	1.41	1.35
2	A	401	1QU	C32-C16	4.22	1.59	1.49
2	B	401	1QU	C11-N2	4.64	1.41	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	1QU	C11-N2-C6	-13.51	103.90	119.25
2	C	401	1QU	C11-N2-C6	-10.39	107.44	119.25
2	C	401	1QU	C9-C10-C6	-6.73	88.94	104.30
2	B	401	1QU	C8-C7-C6	-5.89	90.85	104.30
2	C	401	1QU	C8-C7-C6	-5.38	92.02	104.30
2	C	401	1QU	F1-C32-C16	-5.03	102.19	112.95
2	B	401	1QU	F2-C32-C16	-4.65	103.00	112.95

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	1QU	C9-C10-C6	-3.85	95.52	104.30
2	C	401	1QU	O1-C1-C2	-3.84	117.24	127.09
2	C	401	1QU	C3-C4-N1	-3.75	100.08	103.52
2	A	401	1QU	F1-C32-C16	-3.62	105.21	112.95
2	C	401	1QU	C5-C33-N1	-3.28	115.93	120.16
2	A	401	1QU	C5-C33-N1	-3.18	116.06	120.16
2	C	401	1QU	C4-N1-C33	-3.00	115.62	121.15
2	B	401	1QU	O1-C1-C2	-2.57	120.48	127.09
2	C	401	1QU	F2-C32-C16	-2.47	107.66	112.95
2	B	401	1QU	C18-C19-C14	-2.35	116.91	120.65
2	C	401	1QU	C3-C2-C1	-2.28	97.67	104.57
2	B	401	1QU	C14-C30-N4	-2.22	107.37	112.88
2	B	401	1QU	C31-C27-C28	-2.14	107.49	111.57
2	B	401	1QU	C11-C12-C26	-2.01	113.04	119.60
2	C	401	1QU	C14-C30-N4	-2.01	107.89	112.88
2	B	401	1QU	F3-C32-C16	2.07	117.37	112.95
2	B	401	1QU	C12-C13-C33	2.16	123.07	118.33
2	C	401	1QU	C13-C12-C26	2.42	128.07	120.49
2	B	401	1QU	C13-C12-C26	2.61	128.66	120.49
2	B	401	1QU	C28-C27-N3	2.62	113.94	109.73
2	A	401	1QU	O1-C1-N1	2.79	127.62	125.47
2	A	401	1QU	C7-C6-C10	2.99	107.42	104.32
2	A	401	1QU	C11-N2-C6	3.06	122.72	119.25
2	A	401	1QU	C28-C27-N3	5.06	117.88	109.73
2	B	401	1QU	C7-C6-C10	5.45	109.95	104.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	1QU	3	0
2	C	401	1QU	2	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	370/388 (95%)	0.42	29 (7%)	16 22	26, 45, 84, 116	0
1	B	369/388 (95%)	0.14	7 (1%)	70 76	25, 41, 72, 112	0
1	C	370/388 (95%)	0.10	12 (3%)	51 60	27, 43, 75, 104	0
All	All	1109/1164 (95%)	0.22	48 (4%)	39 48	25, 43, 78, 116	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	THR	5.8
1	A	273	GLY	5.1
1	C	272	ALA	4.7
1	B	10	SER	4.5
1	A	272	ALA	4.4
1	A	317	ASP	4.2
1	A	274	THR	3.9
1	A	271	GLN	3.8
1	A	275	THR	3.6
1	A	257	PHE	3.6
1	C	364	GLU	3.3
1	A	268	VAL	3.1
1	A	309	VAL	3.0
1	A	365	PHE	3.0
1	A	145	HIS	2.9
1	A	270	TRP	2.9
1	C	145	HIS	2.8
1	A	269	CYS	2.8
1	A	319	CYS	2.8
1	A	255	GLU	2.7
1	B	385	ASN	2.6
1	A	256	LYS	2.6
1	A	362	HIS	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	365	PHE	2.6
1	B	317	ASP	2.6
1	C	268	VAL	2.5
1	C	259	ASP	2.5
1	A	253	SER	2.5
1	C	256	LYS	2.4
1	C	10	SER	2.4
1	A	265	GLU	2.4
1	C	273	GLY	2.4
1	B	256	LYS	2.4
1	A	364	GLU	2.3
1	A	278	ASN	2.3
1	C	64	ARG	2.3
1	A	385	ASN	2.3
1	B	365	PHE	2.3
1	A	259	ASP	2.3
1	A	252	SER	2.2
1	A	56	LEU	2.2
1	A	142	LYS	2.2
1	B	269	CYS	2.2
1	A	157	ALA	2.2
1	C	267	LEU	2.1
1	C	270	TRP	2.1
1	A	10	SER	2.0
1	B	22	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	1QU	C	401	44/44	0.96	0.15	1.14	31,36,49,62	0
2	1QU	B	401	44/44	0.97	0.16	0.78	25,34,47,64	0
2	1QU	A	401	44/44	0.97	0.14	-0.35	31,39,52,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.