



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 08:46 AM EDT

PDB ID : 3SKF  
Title : Crystal structure of beta-site app-cleaving enzyme 1 (BACE-WT) complex with (2S)-2-((3S)-3-(acetylamino)-3-(butan-2-yl)-2-oxopyrrolidin-1-yl)-N-((2S,3R)-3-hydroxy-4-((3-methoxybenzyl)amino)-1-phenylbutan-2-yl)-4-phenylbutanamide  
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Deposited on : 2011-06-22  
Resolution : 3.00 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](#) ①) 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
buster-report	:	1.1.7 (2018)
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

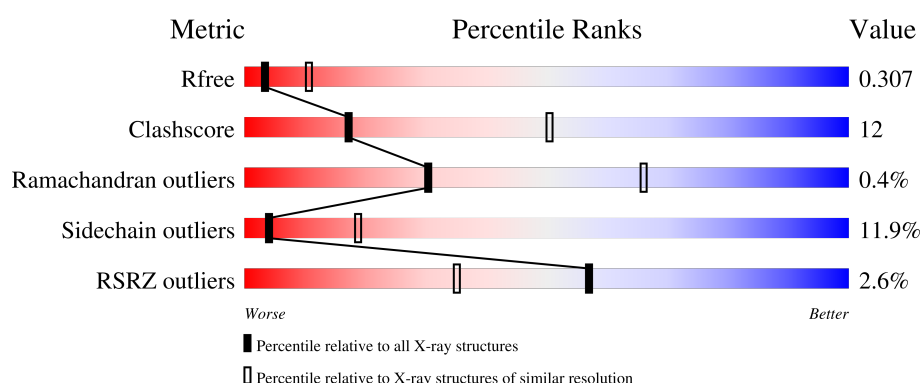
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	455	<div> <div>3%</div> <div>61%</div> <div>20%</div> <div>•</div> <div>15%</div> </div>
1	B	455	<div> <div>2%</div> <div>60%</div> <div>21%</div> <div>• •</div> <div>15%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6361 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	387	Total	C	N	O	S	0	0	0
			3038	1946	505	573	14			
1	B	387	Total	C	N	O	S	0	0	0
			3039	1947	505	573	14			

There are 28 discrepancies between the modelled and reference sequences:

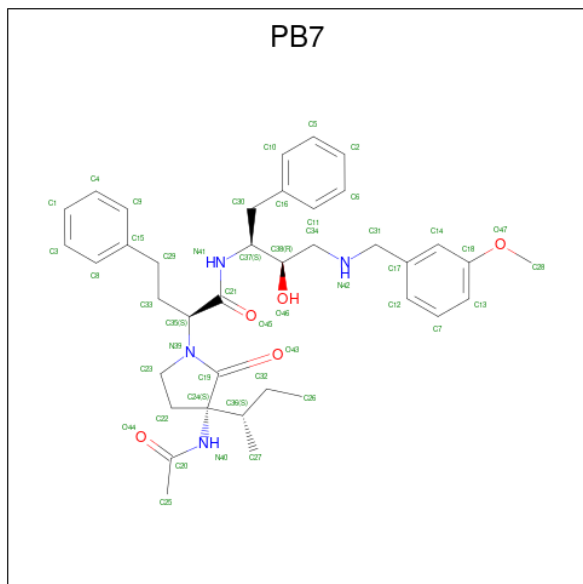
Chain	Residue	Modelled	Actual	Comment	Reference
A	-61	MET	-	expression tag	UNP P56817
A	-60	ALA	-	expression tag	UNP P56817
A	-59	SER	-	expression tag	UNP P56817
A	-58	MET	-	expression tag	UNP P56817
A	-57	THR	-	expression tag	UNP P56817
A	-56	GLY	-	expression tag	UNP P56817
A	-55	GLY	-	expression tag	UNP P56817
A	-54	GLN	-	expression tag	UNP P56817
A	-53	GLN	-	expression tag	UNP P56817
A	-52	MET	-	expression tag	UNP P56817
A	-51	GLY	-	expression tag	UNP P56817
A	-50	ARG	-	expression tag	UNP P56817
A	-49	GLY	-	expression tag	UNP P56817
A	-48	SER	-	expression tag	UNP P56817
B	-61	MET	-	expression tag	UNP P56817
B	-60	ALA	-	expression tag	UNP P56817
B	-59	SER	-	expression tag	UNP P56817
B	-58	MET	-	expression tag	UNP P56817
B	-57	THR	-	expression tag	UNP P56817
B	-56	GLY	-	expression tag	UNP P56817
B	-55	GLY	-	expression tag	UNP P56817
B	-54	GLN	-	expression tag	UNP P56817
B	-53	GLN	-	expression tag	UNP P56817
B	-52	MET	-	expression tag	UNP P56817
B	-51	GLY	-	expression tag	UNP P56817

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-50	ARG	-	expression tag	UNP P56817
B	-49	GLY	-	expression tag	UNP P56817
B	-48	SER	-	expression tag	UNP P56817

- Molecule 2 is (2S)-2-[(3S)-3-(acetylamino)-3-[(2S)-butan-2-yl]-2-oxopyrrolidin-1-yl]-N-[(2S,3R)-3-hydroxy-4-[(3-methoxybenzyl)amino]-1-phenylbutan-2-yl]-4-phenylbutanamide (three-letter code: PB7) (formula: C<sub>38</sub>H<sub>50</sub>N<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			47	38	4	5		
2	B	1	Total	C	N	O	0	0
			47	38	4	5		

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total 89	O 89	0	0
4	B	99	Total 99	O 99	0	0

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.

Chain A:

3% 61% 20% 15%

MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY VAL GLY LEU PRO ALA HIS GLY THR GLN HIS GLY ILE ARG LEU PRO LEU SER GLY LEU GLY ALA PRO LEU LEU LEU ARG LEU PRO ARG GLU THR ASP GLU GLU PRO GLU GLU PRO GLY ARG GLY SER

F-1 V0 E1 M2 L6 G13 V16 E17 V20 G21 S22 Q25 T26 L27 L30 V31 D32 T33 G34 T59 L63 R64 R65 G66 G67 V68 V69 P70 Y71 T72 Q73 W76 L80 G81 V85 G90 Y95 S105 E116 L121 A122 T125 E126

A127 R128 L133 F134 P135 F136 F137 G138 D139 S139 L140 L141 H145 H146 L152 L153 V166 G167 M162 V166 G166 S167 L168 I179 T185 G186 S187 L188 I193 R194 R195 F196 W197 Y198 Y199 Q211 D212 L213 K214 M215 K218 Y222 D223 Y228 S229 R235 K238 A243 T248

E255 G260 E265 Q266 L267 Q271 T274 T275 P276 L279 F280 P281 V282 L285 V286 L287 T292 T299 I300 L301 P302 L306 E310 D311 V312 A313 T314 S315 Q316 F322 A323 I324 S325 Q326 V332 V336 I337 Y342 R349 K350 R351 I352 A355

C359 E364 E371 G372 P373 F374 V375 I376 L377 M379 E380 D381 N385 ILE PRO GLN THR ASP GLU THR

Chain B:

60% 21% 15%

Label	Value
A355	251
V356	252
S357	253
A358	254
C359	255
E364	256
V375	260
L376	265
L377	266
D378	267
M379	268
D381	275
C382	276
N385	279
I386	280
PRO	281
GLN	282
THR	285
ASP	285
GLU	292
SER	292
THR	295
T299	299
I300	300
L301	301
P302	302
L306	306
R307	307
P308	308
D311	311
V312	312
A313	313
T314	314
S315	315
Q316	316
S325	325
V332	332
T337	337
M338	338
E339	339
D346	346
R347	347
A348	348
R349	349
R351	351
I352	352

Label	Value
L133	133
F-1	133
V0	134
E1	140
M2	141
V3	146
L6	147
N148	148
S10	149
G13	152
ARG	152
V16	153
V20	154
Q25	165
T26	166
L27	167
L30	174
D32	180
T33	183
G34	184
H49	185
I59	186
T59	187
V67	188
Y68	194
V69	195
P70	196
Y71	197
T72	198
Q73	199
W76	202
L80	211
H89	212
G90	213
V95	214
M114	215
W115	216
E116	218
G119	222
G120	223
L121	229
E125	233
I126	234
A127	235
R128	243
E128	244

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.29Å 130.26Å 85.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.06 – 3.00 34.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.06-3.00) 99.4 (34.06-3.00)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.252 , 0.313 0.252 , 0.307	Depositor DCC
$R_{free}$ test set	1064 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0775e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, PB7

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	0.48	1/3116 (0.0%)	0.64	1/4238 (0.0%)
1	B	0.48	1/3117 (0.0%)	0.65	2/4239 (0.0%)
All	All	0.48	2/6233 (0.0%)	0.65	3/8477 (0.0%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	CYS	CB-SG	-6.54	1.71	1.82
1	B	359	CYS	CB-SG	-5.17	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	LEU	CA-CB-CG	6.85	131.06	115.30
1	B	140	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	267	LEU	CA-CB-CG	5.22	127.30	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	379	MET	Peptide
1	B	380	GLU	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	3038	0	2950	76	0
1	B	3039	0	2952	80	0
2	A	47	0	50	2	0
2	B	47	0	50	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	89	0	0	5	0
4	B	99	0	0	2	0
All	All	6361	0	6002	151	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 12.

All (151) 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:B:254:THR:HB	1:B:279:ILE:HD11	1.24	1.18
1:A:276:PRO:O	1:A:279:ILE:HG22	1.63	0.96
1:A:235:ARG:HB2	1:A:332:VAL:HG23	1.47	0.95
1:B:67:VAL:HB	1:B:80:LEU:HD21	1.50	0.94
1:B:276:PRO:O	1:B:279:ILE:HG22	1.73	0.88
1:B:235:ARG:HB2	1:B:332:VAL:HG12	1.59	0.84
1:A:67:VAL:HB	1:A:80:LEU:HD21	1.61	0.80
1:B:254:THR:HB	1:B:279:ILE:CD1	2.12	0.77
1:B:13:GLY:HA3	1:B:30:LEU:HD11	1.70	0.74
1:A:310:GLU:HG2	4:A:481:HOH:O	1.91	0.71
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.72	0.70
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.73	0.69
1:B:188:LEU:HD13	1:B:355:ALA:HB2	1.75	0.69
1:B:295:SER:CB	1:B:377:LEU:HD23	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:VAL:HG13	1:B:299:THR:HG23	1.77	0.66
1:A:34:GLY:O	2:A:394:PB7:H14	1.95	0.66
1:A:6:LEU:HD12	1:A:16:VAL:HG12	1.78	0.66
1:A:67:VAL:HB	1:A:80:LEU:CD2	2.25	0.66
1:A:379:MET:O	1:A:379:MET:CG	2.43	0.66
1:A:140:LEU:HD13	1:A:146:VAL:HG11	1.79	0.65
1:A:276:PRO:HB2	1:A:279:ILE:CG2	2.28	0.64
1:A:379:MET:O	1:A:379:MET:HG3	1.99	0.63
1:A:276:PRO:HB2	1:A:279:ILE:HG22	1.80	0.63
1:A:22:SER:HB2	1:A:59:THR:OG1	2.01	0.61
1:B:33:THR:H	1:B:229:SER:HB3	1.66	0.60
1:B:197:TRP:H	1:B:197:TRP:HD1	1.47	0.60
1:A:33:THR:H	1:A:229:SER:CB	2.15	0.60
1:A:282:VAL:HG13	1:A:299:THR:HG23	1.84	0.60
1:A:235:ARG:HB2	1:A:332:VAL:CG2	2.29	0.60
1:A:188:LEU:HD13	1:A:355:ALA:HB2	1.85	0.59
1:B:380:GLU:C	1:B:382:CYS:H	2.05	0.59
1:B:69:VAL:HG22	1:B:128:ARG:HB2	1.85	0.59
1:A:300:ILE:HD13	1:A:337:ILE:HD12	1.84	0.58
1:B:33:THR:H	1:B:229:SER:CB	2.15	0.58
1:A:95:VAL:HG11	1:A:140:LEU:HA	1.86	0.57
1:B:295:SER:CB	1:B:377:LEU:CD2	2.83	0.56
1:B:6:LEU:HD11	1:B:174:MET:HB2	1.87	0.56
1:A:69:VAL:HG22	1:A:128:ARG:HB2	1.88	0.56
1:A:125:GLU:OE2	1:A:195:ARG:NH2	2.38	0.55
1:B:125:GLU:OE2	1:B:195:ARG:NH2	2.37	0.54
1:A:197:TRP:H	1:A:197:TRP:HD1	1.55	0.54
1:B:180:ASP:HB3	1:B:183:LEU:HD22	1.89	0.54
1:B:375:VAL:O	1:B:377:LEU:N	2.39	0.54
1:A:64:ARG:NE	4:A:420:HOH:O	2.40	0.54
1:B:148:ASN:HB3	1:B:348:ALA:HB2	1.91	0.53
1:A:179:ILE:HG23	1:A:342:TYR:HE2	1.74	0.53
1:A:375:VAL:O	1:A:377:LEU:N	2.41	0.53
1:A:376:THR:OG1	1:B:364:GLU:CD	2.47	0.53
1:B:89:HIS:HD2	4:B:457:HOH:O	1.92	0.52
1:A:199:TYR:HB3	1:A:352:ILE:HD11	1.92	0.52
1:A:248:ILE:HG13	1:A:281:PRO:HG2	1.91	0.51
1:B:32:ASP:HA	1:B:229:SER:HB3	1.92	0.51
1:A:271:GLN:O	1:A:274:THR:HB	2.11	0.51
1:B:13:GLY:HA3	1:B:30:LEU:CD1	2.40	0.51
1:B:199:TYR:HB3	1:B:352:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:CD1	1:B:174:MET:HB2	2.41	0.51
1:B:67:VAL:HB	1:B:80:LEU:CD2	2.33	0.50
1:B:295:SER:HB3	1:B:377:LEU:CD2	2.42	0.50
1:B:295:SER:HB2	1:B:377:LEU:HD23	1.94	0.50
1:A:33:THR:H	1:A:229:SER:HB3	1.75	0.50
1:B:34:GLY:O	2:B:394:PB7:H14	2.12	0.50
1:A:364:GLU:OE2	1:B:376:THR:N	2.40	0.49
1:A:33:THR:H	1:A:229:SER:HB2	1.76	0.49
1:B:260:GLY:C	1:B:266:GLN:HB3	2.32	0.49
1:A:6:LEU:CD1	1:A:16:VAL:HG12	2.41	0.49
1:B:27:LEU:HD22	1:B:116:GLU:HG3	1.94	0.49
1:A:13:GLY:HA3	1:A:30:LEU:CD1	2.42	0.49
1:A:279:ILE:HA	1:B:211:GLN:HG3	1.94	0.49
1:A:63:LEU:HD22	1:A:81:GLY:HA2	1.95	0.48
1:B:194:ARG:HG3	1:B:202:ILE:HD11	1.95	0.48
1:B:119:LEU:HG	1:B:121:LEU:HD22	1.95	0.48
1:A:13:GLY:HA3	1:A:30:LEU:HD11	1.94	0.48
2:A:394:PB7:H32A	2:A:394:PB7:O43	2.13	0.48
1:B:301:LEU:HB3	1:B:302:PRO:HD2	1.96	0.48
1:A:302:PRO:O	1:A:306:LEU:HB2	2.14	0.47
1:A:228:ASP:HB3	1:A:332:VAL:HG12	1.95	0.47
1:A:2:MET:CG	1:A:90:GLY:HA2	2.42	0.47
1:A:152:LEU:CD1	1:A:174:MET:HG3	2.45	0.47
1:B:215:MET:CE	1:B:243:ALA:HB3	2.44	0.47
1:A:135:PRO:HD2	1:A:138:ASP:OD2	2.15	0.47
1:B:375:VAL:C	1:B:377:LEU:H	2.18	0.46
1:A:375:VAL:C	1:A:377:LEU:H	2.19	0.46
1:B:71:TYR:HE2	1:B:76:TRP:HE1	1.62	0.46
1:B:222:TYR:HA	1:B:223:ASP:HA	1.69	0.46
1:B:300:ILE:HD13	1:B:337:ILE:HD12	1.98	0.46
1:A:248:ILE:HG13	1:A:281:PRO:CG	2.46	0.46
1:A:222:TYR:HA	1:A:223:ASP:HA	1.72	0.46
1:A:336:VAL:HG12	1:A:337:ILE:HD13	1.98	0.46
1:B:149:LEU:HD22	1:B:346:ASP:HA	1.98	0.46
1:B:248:ILE:HG13	1:B:281:PRO:CG	2.46	0.46
1:A:27:LEU:HD22	1:A:116:GLU:HG3	1.98	0.45
1:B:349:ARG:HH11	1:B:351:ARG:NH2	2.13	0.45
1:B:188:LEU:HD13	1:B:355:ALA:CB	2.43	0.45
1:A:32:ASP:HA	1:A:229:SER:HB3	1.97	0.45
1:A:6:LEU:HD11	1:A:174:MET:HB2	1.98	0.45
1:B:282:VAL:CG1	1:B:299:THR:HG23	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:MET:HG2	1:B:380:GLU:HB3	1.99	0.45
1:B:233:ASN:HD22	1:B:325:SER:HB3	1.81	0.44
1:A:6:LEU:CD1	1:A:174:MET:HB2	2.47	0.44
1:B:282:VAL:HG13	1:B:299:THR:CG2	2.47	0.44
1:A:65:LYS:HE2	4:A:473:HOH:O	2.17	0.44
1:B:10:SER:HB3	1:B:339:GLU:OE2	2.16	0.44
1:A:322:PHE:CE2	1:A:324:ILE:HB	2.53	0.44
1:B:380:GLU:C	1:B:382:CYS:N	2.71	0.44
1:B:67:VAL:HG12	1:B:80:LEU:HD22	1.99	0.44
1:B:235:ARG:HG3	1:B:332:VAL:CG1	2.48	0.43
1:B:302:PRO:O	1:B:306:LEU:HB2	2.18	0.43
1:A:218:LYS:HG3	1:A:381:ASP:O	2.17	0.43
1:B:69:VAL:HG22	1:B:128:ARG:CB	2.47	0.43
1:B:114:ASN:HD22	1:B:167:LEU:CD2	2.31	0.43
1:A:33:THR:HG23	1:A:229:SER:HB2	2.00	0.43
1:A:16:VAL:HG13	1:A:31:VAL:CG2	2.48	0.43
1:A:85:VAL:CG1	1:A:136:PHE:HE1	2.31	0.43
1:B:254:THR:CB	1:B:279:ILE:HD11	2.18	0.43
1:A:211:GLN:HG3	1:B:279:ILE:HA	2.01	0.43
1:A:85:VAL:HG12	1:A:95:VAL:O	2.19	0.42
1:A:275:THR:HA	1:A:276:PRO:HD3	1.85	0.42
1:A:349:ARG:HH11	1:A:351:ARG:NH2	2.17	0.42
1:B:68:TYR:CD2	1:B:70:PRO:HD3	2.54	0.42
1:A:260:GLY:C	1:A:266:GLN:HB3	2.40	0.42
1:A:85:VAL:HG11	1:A:136:PHE:HE1	1.83	0.42
1:B:20:VAL:O	1:B:25:GLN:HB2	2.19	0.42
1:B:379:MET:O	1:B:380:GLU:HG3	2.20	0.42
1:B:140:LEU:CD1	1:B:146:VAL:HG11	2.50	0.42
1:B:250:ALA:O	1:B:253:SER:OG	2.38	0.42
1:B:308:PRO:HD2	4:B:398:HOH:O	2.20	0.42
1:B:256:LYS:HD3	1:B:256:LYS:HA	1.88	0.42
1:A:122:ALA:HA	1:A:199:TYR:CE2	2.55	0.42
1:A:193:ILE:HB	1:A:350:LYS:HG2	2.01	0.42
1:A:17:GLU:HB3	4:A:445:HOH:O	2.20	0.41
1:A:20:VAL:O	1:A:25:GLN:HB2	2.19	0.41
1:A:238:LYS:CG	1:A:326:GLN:NE2	2.84	0.41
1:A:364:GLU:CD	1:B:376:THR:OG1	2.58	0.41
1:A:16:VAL:HG13	1:A:31:VAL:HG23	2.03	0.41
1:A:71:TYR:HE2	1:A:76:TRP:HE1	1.67	0.41
1:A:238:LYS:HG3	1:A:326:GLN:NE2	2.35	0.41
1:B:146:VAL:HA	1:B:147:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:HG2	4:A:458:HOH:O	2.21	0.41
1:B:152:LEU:CD1	1:B:174:MET:HG3	2.50	0.41
1:B:197:TRP:CD1	1:B:197:TRP:N	2.83	0.41
1:A:71:TYR:HE2	1:A:76:TRP:NE1	2.18	0.41
1:A:215:MET:HE3	1:A:243:ALA:HB3	2.02	0.41
1:B:248:ILE:HG13	1:B:281:PRO:HG2	2.03	0.41
1:B:215:MET:HE3	1:B:243:ALA:HB3	2.02	0.40
1:B:218:LYS:HG3	1:B:381:ASP:O	2.22	0.40
1:B:275:THR:HA	1:B:276:PRO:HD3	1.88	0.40
1:A:376:THR:HG23	1:B:364:GLU:OE1	2.21	0.40
1:B:68:TYR:CE2	1:B:70:PRO:HD3	2.56	0.40
1:B:140:LEU:HD13	1:B:146:VAL:HG11	2.04	0.40
1:B:72:THR:OG1	2:B:394:PB7:H12	2.21	0.40
1:B:154:LEU:O	1:B:339:GLU:HA	2.21	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	385/455 (85%)	366 (95%)	18 (5%)	1 (0%)	37	70
1	B	385/455 (85%)	363 (94%)	20 (5%)	2 (0%)	25	61
All	All	770/910 (85%)	729 (95%)	38 (5%)	3 (0%)	30	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	THR
1	B	376	THR
1	B	380	GLU

### 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	329/381 (86%)	289 (88%)	40 (12%)	4	18
1	B	329/381 (86%)	291 (88%)	38 (12%)	4	20
All	All	658/762 (86%)	580 (88%)	78 (12%)	4	19

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	VAL
1	A	59	THR
1	A	63	LEU
1	A	73	GLN
1	A	95	VAL
1	A	105	SER
1	A	116	GLU
1	A	121	LEU
1	A	126	ILE
1	A	133	LEU
1	A	140	LEU
1	A	141	VAL
1	A	145	HIS
1	A	146	VAL
1	A	166	VAL
1	A	185	THR
1	A	187	SER
1	A	188	LEU
1	A	197	TRP
1	A	213	LEU
1	A	229	SER
1	A	248	ILE
1	A	255	GLU
1	A	265	GLU
1	A	279	ILE
1	A	282	VAL
1	A	285	LEU

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Mol	Chain	Res	Type
1	A	287	LEU
1	A	292	THR
1	A	301	LEU
1	A	306	LEU
1	A	316	GLN
1	A	332	VAL
1	A	359	CYS
1	A	364	GLU
1	A	373	PRO
1	A	376	THR
1	A	377	LEU
1	A	378	ASP
1	A	379	MET
1	B	0	VAL
1	B	3	VAL
1	B	16	VAL
1	B	49	HIS
1	B	59	THR
1	B	73	GLN
1	B	89	HIS
1	B	95	VAL
1	B	116	GLU
1	B	126	ILE
1	B	133	LEU
1	B	140	LEU
1	B	141	VAL
1	B	146	VAL
1	B	149	LEU
1	B	152	LEU
1	B	165	GLU
1	B	167	LEU
1	B	183	LEU
1	B	185	THR
1	B	187	SER
1	B	197	TRP
1	B	213	LEU
1	B	234	LEU
1	B	252	SER
1	B	253	SER
1	B	265	GLU
1	B	268	VAL
1	B	282	VAL

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Mol	Chain	Res	Type
1	B	285	LEU
1	B	292	THR
1	B	306	LEU
1	B	316	GLN
1	B	357	SER
1	B	359	CYS
1	B	376	THR
1	B	377	LEU
1	B	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
1	B	28	ASN
1	B	89	HIS
1	B	114	ASN

### 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	PB7	A	394	-	50,50,50	5.79	28 (56%)	57,68,68	1.11	4 (7%)
2	PB7	B	394	-	50,50,50	5.86	28 (56%)	57,68,68	1.27	6 (10%)

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	PB7	A	394	-	-	7/46/62/62	0/4/4/4
2	PB7	B	394	-	-	5/46/62/62	0/4/4/4

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	394	PB7	O43-C19	13.46	1.42	1.22
2	B	394	PB7	O43-C19	13.43	1.42	1.22
2	B	394	PB7	O45-C21	10.58	1.43	1.23
2	A	394	PB7	O45-C21	10.01	1.42	1.23
2	A	394	PB7	C19-N39	9.12	1.49	1.34
2	B	394	PB7	O44-C20	9.11	1.43	1.23
2	B	394	PB7	C7-C13	8.86	1.54	1.38
2	A	394	PB7	C7-C13	8.71	1.53	1.38
2	A	394	PB7	C5-C10	8.70	1.53	1.38
2	B	394	PB7	C20-N40	8.67	1.48	1.34
2	A	394	PB7	O44-C20	8.66	1.42	1.23
2	B	394	PB7	C7-C12	8.65	1.53	1.38
2	A	394	PB7	C7-C12	8.58	1.53	1.38
2	A	394	PB7	C20-N40	8.57	1.48	1.34
2	B	394	PB7	C14-C18	8.56	1.53	1.39
2	B	394	PB7	C4-C9	8.48	1.53	1.38
2	A	394	PB7	C14-C17	8.46	1.53	1.39
2	B	394	PB7	C14-C17	8.45	1.53	1.39
2	A	394	PB7	C14-C18	8.42	1.52	1.39
2	B	394	PB7	C19-N39	8.34	1.48	1.34
2	B	394	PB7	C13-C18	8.34	1.54	1.38
2	B	394	PB7	C3-C8	8.34	1.53	1.38
2	B	394	PB7	C5-C10	8.33	1.53	1.38
2	A	394	PB7	C6-C11	8.32	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	394	PB7	C6-C11	8.24	1.53	1.38
2	A	394	PB7	C3-C8	8.21	1.52	1.38
2	A	394	PB7	C4-C9	8.20	1.52	1.38
2	A	394	PB7	C13-C18	7.87	1.53	1.38
2	B	394	PB7	C21-N41	7.65	1.50	1.34
2	B	394	PB7	C8-C15	7.54	1.53	1.38
2	A	394	PB7	C10-C16	7.38	1.53	1.38
2	B	394	PB7	C11-C16	7.34	1.53	1.38
2	B	394	PB7	C12-C17	7.26	1.53	1.38
2	B	394	PB7	C10-C16	7.25	1.53	1.38
2	A	394	PB7	C12-C17	7.20	1.53	1.38
2	B	394	PB7	C9-C15	7.08	1.52	1.38
2	B	394	PB7	C4-C1	7.07	1.53	1.38
2	A	394	PB7	C11-C16	7.04	1.52	1.38
2	A	394	PB7	C8-C15	7.03	1.52	1.38
2	A	394	PB7	C21-N41	7.01	1.49	1.34
2	A	394	PB7	C6-C2	6.96	1.53	1.38
2	A	394	PB7	C9-C15	6.94	1.52	1.38
2	B	394	PB7	C3-C1	6.87	1.53	1.38
2	B	394	PB7	C6-C2	6.86	1.53	1.38
2	A	394	PB7	C5-C2	6.82	1.53	1.38
2	B	394	PB7	C5-C2	6.79	1.53	1.38
2	A	394	PB7	C4-C1	6.68	1.52	1.38
2	A	394	PB7	C3-C1	6.59	1.52	1.38
2	A	394	PB7	C35-N39	3.67	1.50	1.46
2	B	394	PB7	O47-C18	3.32	1.44	1.37
2	A	394	PB7	O47-C18	3.18	1.43	1.37
2	B	394	PB7	C24-N40	2.76	1.50	1.45
2	B	394	PB7	C35-N39	2.59	1.49	1.46
2	A	394	PB7	C24-N40	2.57	1.49	1.45
2	A	394	PB7	C37-N41	2.48	1.50	1.46
2	B	394	PB7	C37-N41	2.13	1.49	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	394	PB7	C23-N39-C19	-3.69	111.12	113.47
2	A	394	PB7	C27-C36-C32	-3.56	107.25	110.83
2	B	394	PB7	O44-C20-N40	3.45	127.01	122.23
2	B	394	PB7	C27-C36-C32	-3.41	107.40	110.83
2	A	394	PB7	C23-N39-C19	-3.03	111.54	113.47
2	B	394	PB7	C25-C20-N40	-2.82	112.43	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	394	PB7	C30-C37-C38	2.31	115.41	111.66
2	B	394	PB7	C24-N40-C20	2.16	125.44	121.31
2	A	394	PB7	C35-N39-C19	2.08	124.60	122.12
2	B	394	PB7	C22-C23-N39	-2.00	101.06	103.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	394	PB7	C22-C24-C36-C32
2	B	394	PB7	N42-C34-C38-O46
2	A	394	PB7	C13-C18-O47-C28
2	A	394	PB7	C14-C18-O47-C28
2	B	394	PB7	C17-C31-N42-C34
2	B	394	PB7	N42-C34-C38-C37
2	B	394	PB7	C21-C35-N39-C23
2	A	394	PB7	C19-C24-C36-C32
2	A	394	PB7	C33-C35-N39-C23
2	B	394	PB7	C33-C35-N39-C23
2	A	394	PB7	C10-C16-C30-C37
2	A	394	PB7	C11-C16-C30-C37

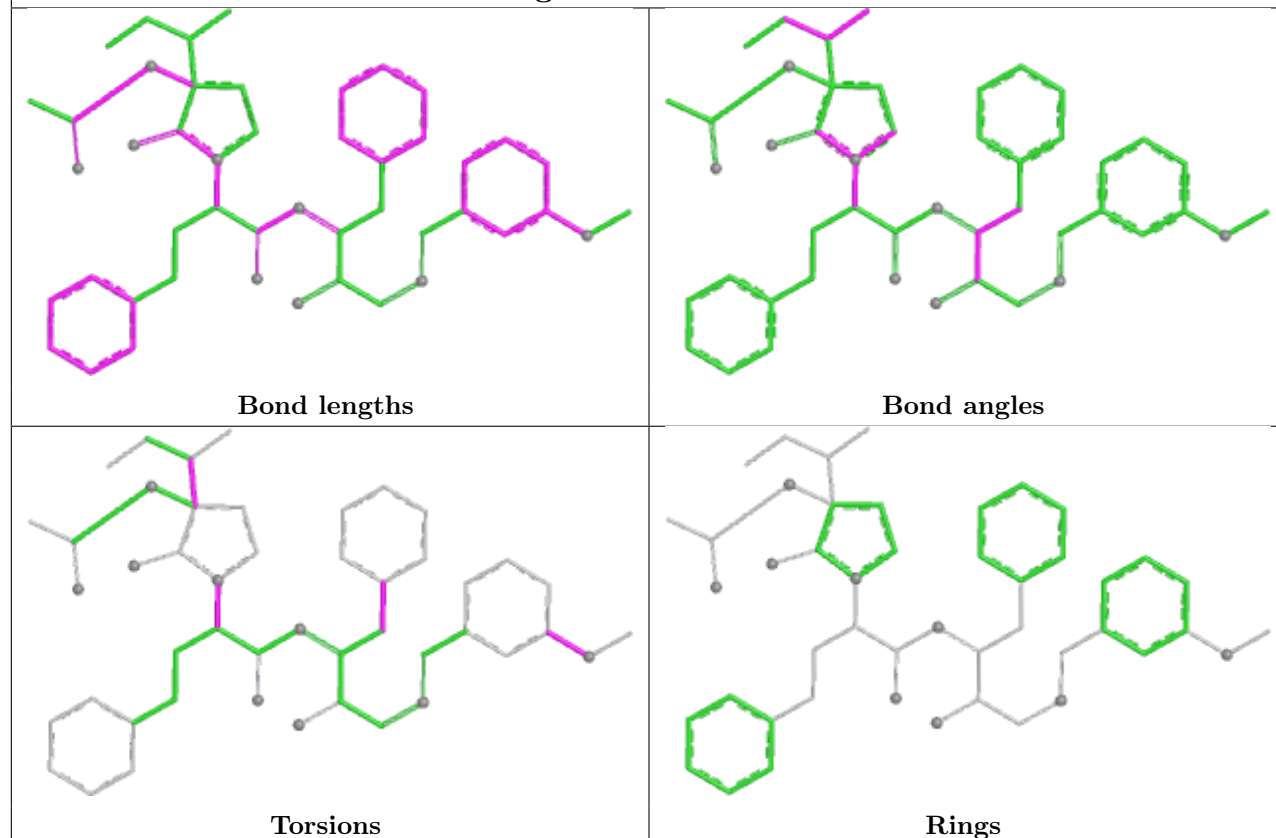
There are no ring outliers.

2 monomers are involved in 4 short contacts:

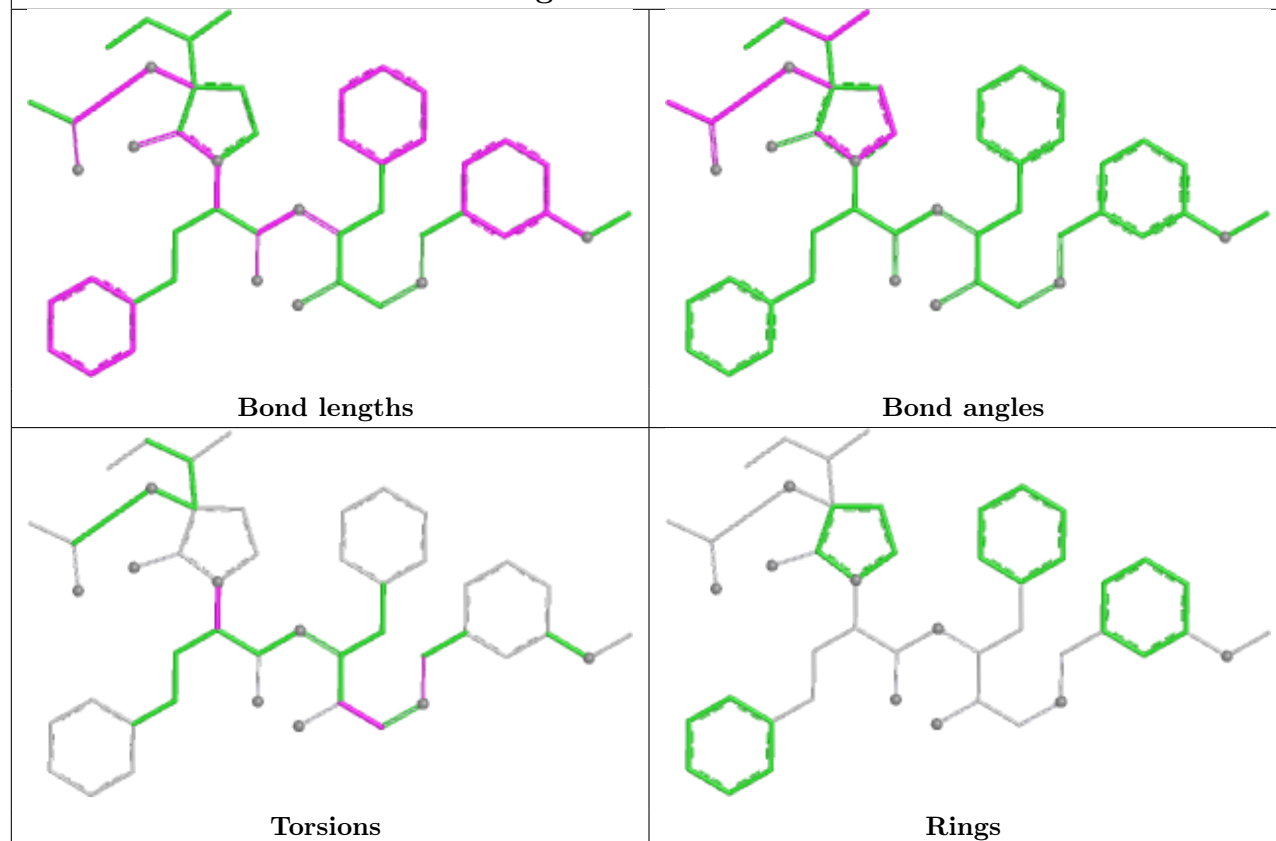
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	394	PB7	2	0
2	B	394	PB7	2	0

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.

## Ligand PB7 A 394



## Ligand PB7 B 394



## 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, 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	387/455 (85%)	0.03	13 (3%) 48 28	22, 32, 35, 36	0
1	B	387/455 (85%)	0.04	7 (1%) 67 45	22, 32, 35, 36	0
All	All	774/910 (85%)	0.04	20 (2%) 57 35	22, 32, 35, 36	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	THR	5.0
1	A	314	THR	3.6
1	A	312	VAL	3.4
1	B	315	SER	3.2
1	A	313	ALA	3.2
1	B	376	THR	2.8
1	B	312	VAL	2.8
1	A	379	MET	2.8
1	A	266	GLN	2.7
1	A	145	HIS	2.6
1	A	364	GLU	2.6
1	A	377	LEU	2.5
1	B	311	ASP	2.5
1	A	315	SER	2.4
1	A	378	ASP	2.4
1	B	364	GLU	2.2
1	A	375	VAL	2.2
1	B	377	LEU	2.2
1	A	376	THR	2.0
1	A	162	ASN	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.

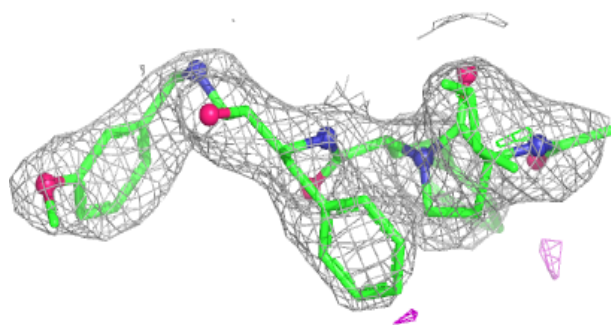
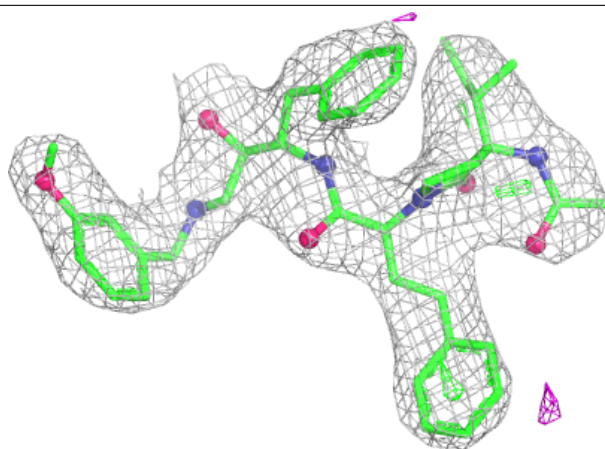
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	IOD	B	395	1/1	0.59	0.30	294,294,294,294	0
3	IOD	A	395	1/1	0.66	0.30	233,233,233,233	0
2	PB7	A	394	47/47	0.91	0.16	30,31,32,32	0
2	PB7	B	394	47/47	0.93	0.13	30,31,32,32	0

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.

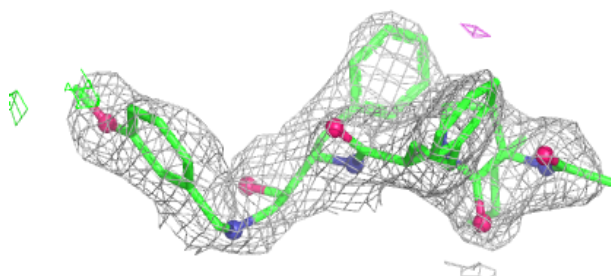
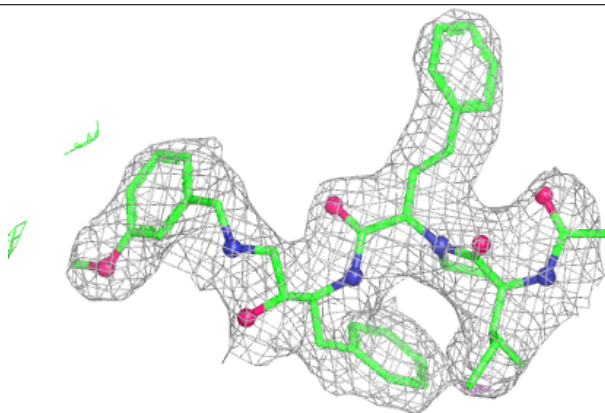


**Electron density around PB7 A 394:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PB7 B 394:**

$2mF_o-DF_c$  (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.