



## Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2024 – 02:25 AM EST

PDB ID : 3R2F  
Title : Crystal structure of beta-site app-cleaving enzyme 1 (BACE-WT) complex with BMS-693391 AKA (2S)-2-((3R)-3-acetamido-3-isobutyl-2-oxo-1-pyrrolidinyl)-N-((1S,2R)-1-(3,5-difluorobenzyl)-2-hydroxy-2-((2R,4R)-4-propoxy-2-pyrrolidinyl)ethyl)-4-phenylbutanamide  
Authors : Muckelbauer, J.K.  
Deposited on : 2011-03-14  
Resolution : 2.53 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

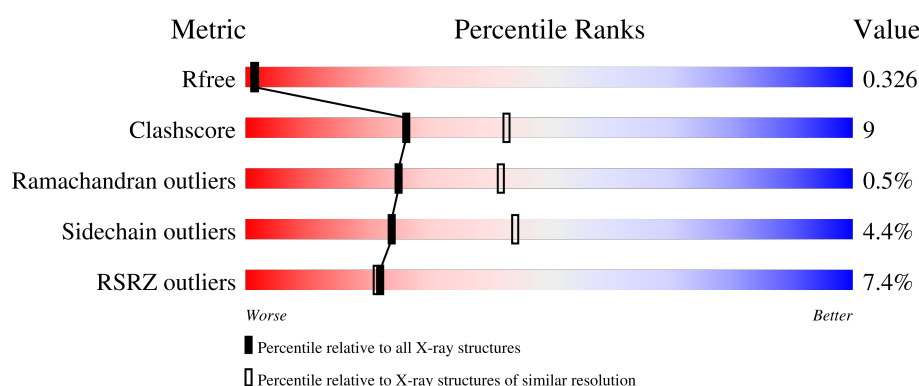
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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	6935 (2.54-2.50)
Clashscore	180529	7778 (2.54-2.50)
Ramachandran outliers	177936	7674 (2.54-2.50)
Sidechain outliers	177891	7676 (2.54-2.50)
RSRZ outliers	164620	6935 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	455	
1	D	455	
1	E	455	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12446 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	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			
1	B	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			
1	D	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			
1	E	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			

There are 56 discrepancies between the modelled and reference sequences:

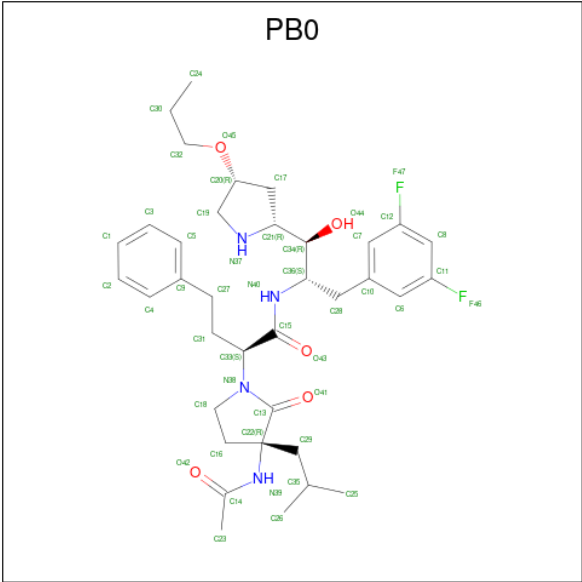
Chain	Residue	Modelled	Actual	Comment	Reference
A	-61	MET	-	expression tag	UNP P56817
A	-60	ALA	-	expression tag	UNP P56817
A	-59	SER	-	expression tag	UNP P56817
A	-58	MET	-	expression tag	UNP P56817
A	-57	THR	-	expression tag	UNP P56817
A	-56	GLY	-	expression tag	UNP P56817
A	-55	GLY	-	expression tag	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

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

- Molecule 2 is (2S)-2-[(3R)-3-(acetylamino)-3-(2-methylpropyl)-2-oxopyrrolidin-1-yl]-N-[(1R,2S)-3-(3,5-difluorophenyl)-1-hydroxy-1-[(2R,4R)-4-propoxypyrrolidin-2-yl]propan-2-yl]-4-phenylbutanamide (three-letter code: PB0) (formula: C<sub>36</sub>H<sub>50</sub>F<sub>2</sub>N<sub>4</sub>O<sub>5</sub>).

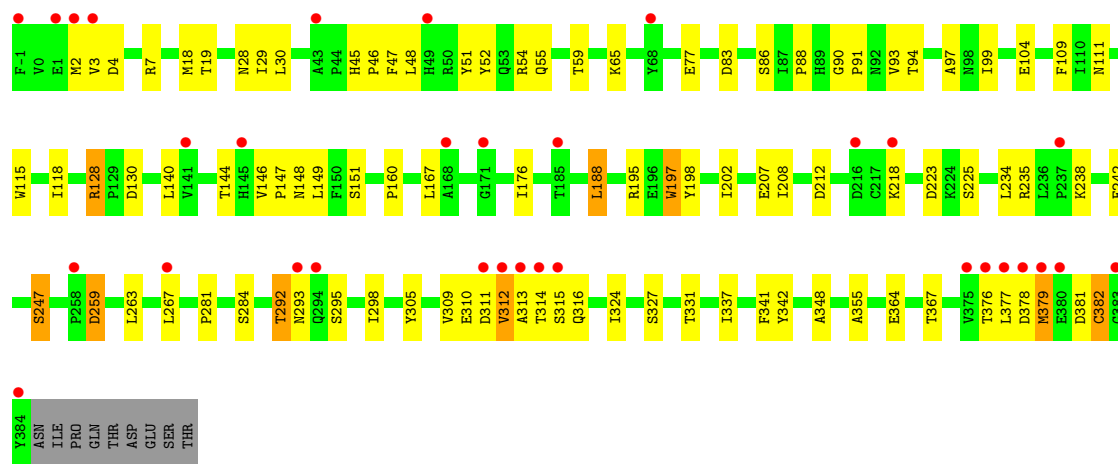


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			47	36	2	4	5		
2	B	1	Total	C	F	N	O	0	0
			47	36	2	4	5		
2	D	1	Total	C	F	N	O	0	0
			47	36	2	4	5		
2	E	1	Total	C	F	N	O	0	0
			47	36	2	4	5		

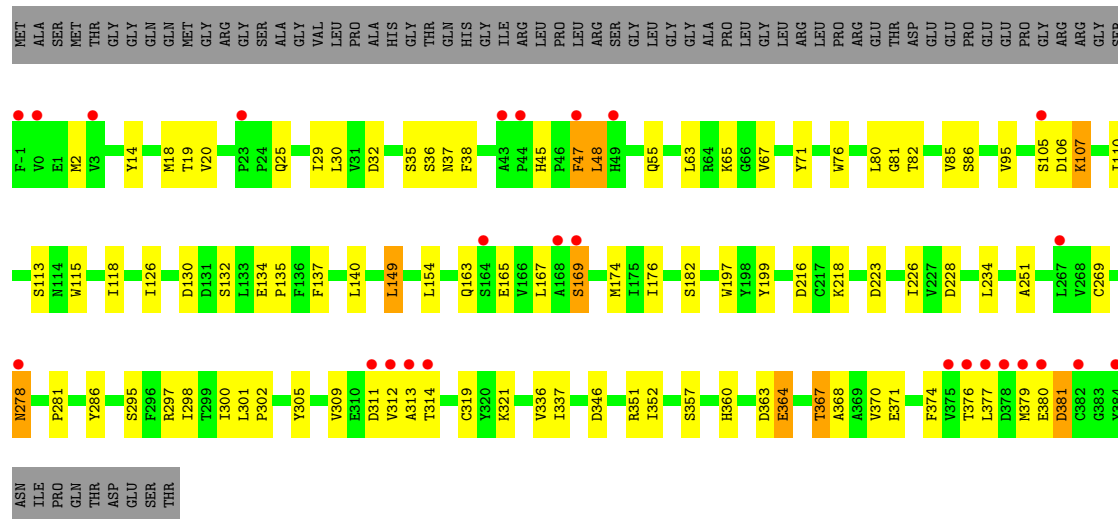
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	44	Total	O	0	0
			44	44		
3	D	22	Total	O	0	0
			22	22		
3	E	28	Total	O	0	0
			28	28		





• 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, $\alpha$ , $\beta$ , $\gamma$	86.31Å 130.25Å 86.93Å 90.00° 96.53° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.53 86.36 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.6 ((Not available)-2.53) 98.7 (86.36-2.53)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.0, CNS	Depositor
R, $R_{free}$	0.280 , 0.330 0.279 , 0.326	Depositor DCC
$R_{free}$ test set	3194 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	1.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	12446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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 27.38 % 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 2.2212e-03. 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: PB0

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	0.56	1/3112 (0.0%)	0.69	4/4232 (0.1%)
1	B	0.52	1/3112 (0.0%)	0.65	2/4232 (0.0%)
1	D	0.55	0/3112	0.69	1/4232 (0.0%)
1	E	0.50	0/3112	0.68	4/4232 (0.1%)
All	All	0.53	2/12448 (0.0%)	0.68	11/16928 (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	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378	ASP	C-O	-10.41	1.03	1.23
1	B	131	ASP	C-O	-7.64	1.08	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ASP	CA-C-N	7.38	133.44	117.20
1	E	48	LEU	N-CA-C	6.79	129.35	111.00
1	E	47	PHE	C-N-CA	6.78	138.66	121.70
1	A	378	ASP	O-C-N	-6.11	112.92	122.70
1	B	131	ASP	CA-C-N	5.67	129.68	117.20
1	D	379	MET	N-CA-C	-5.62	95.83	111.00
1	B	131	ASP	O-C-N	-5.62	113.72	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	GLU	N-CA-C	5.49	125.81	111.00
1	A	359	CYS	CA-CB-SG	5.31	123.56	114.00
1	E	278	ASN	N-CA-CB	-5.15	101.33	110.60
1	E	47	PHE	N-CA-C	5.04	124.60	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	47	PHE	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	3034	0	2948	32	4
1	B	3034	0	2950	43	3
1	D	3034	0	2950	73	4
1	E	3034	0	2950	74	3
2	A	47	0	50	0	0
2	B	47	0	50	6	0
2	D	47	0	50	1	0
2	E	47	0	50	6	0
3	A	28	0	0	0	0
3	B	44	0	0	2	0
3	D	22	0	0	1	0
3	E	28	0	0	1	0
All	All	12446	0	11998	222	7

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 9.

All (222) 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:E:163:GLN:O	1:E:167:LEU:HD12	1.33	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LYS:HE2	1:A:381:ASP:O	1.52	1.08
1:D:140:LEU:O	1:D:144:THR:HG22	1.57	1.04
1:D:234:LEU:HB2	1:D:337:ILE:HD11	1.47	0.96
1:D:128:ARG:HG3	1:D:128:ARG:HH11	1.31	0.95
1:D:128:ARG:HH11	1:D:128:ARG:CG	1.84	0.91
1:B:130:ASP:OD1	1:B:132:SER:HB3	1.74	0.88
1:B:131:ASP:O	1:B:132:SER:CB	2.19	0.85
1:E:234:LEU:HB2	1:E:337:ILE:CD1	2.06	0.85
1:D:376:THR:HA	3:D:415:HOH:O	1.76	0.83
1:E:165:GLU:O	1:E:169:SER:OG	1.96	0.82
1:D:281:PRO:O	1:D:305:TYR:OH	1.98	0.81
1:A:165:GLU:O	1:A:169:SER:OG	1.97	0.81
1:E:2:MET:HE1	1:E:176:ILE:H	1.43	0.81
1:D:238:LYS:O	1:D:242:GLU:HG3	1.83	0.79
1:E:269:CYS:HG	1:E:319:CYS:HG	0.79	0.78
1:B:194:ARG:HD2	1:B:202:ILE:HD11	1.64	0.78
1:E:45:HIS:HB3	1:E:48:LEU:HB2	1.67	0.77
1:E:218:LYS:HE3	1:E:381:ASP:O	1.85	0.76
1:E:234:LEU:HB2	1:E:337:ILE:HD11	1.68	0.76
1:D:19:THR:OG1	1:D:86:SER:HB2	1.86	0.76
1:E:298:ILE:HG22	1:E:370:VAL:HG22	1.68	0.75
1:D:267:LEU:HD22	1:D:309:VAL:HG21	1.69	0.74
1:D:311:ASP:OD1	1:D:312:VAL:CG2	2.36	0.73
1:E:65:LYS:HE3	1:E:80:LEU:HD12	1.72	0.72
1:B:269:CYS:HG	1:B:319:CYS:HG	1.37	0.71
1:A:378:ASP:O	1:A:379:MET:HB2	1.91	0.70
1:B:131:ASP:O	1:B:132:SER:HB3	1.90	0.70
1:D:2:MET:HE3	1:D:90:GLY:HA2	1.73	0.69
1:A:234:LEU:HB2	1:A:337:ILE:HD11	1.73	0.68
1:E:63:LEU:HD21	1:E:82:THR:HG23	1.74	0.68
1:E:174:MET:CE	1:E:176:ILE:HD11	2.24	0.68
1:E:234:LEU:HB2	1:E:337:ILE:HD13	1.75	0.67
2:D:394:PB0:H26	2:D:394:PB0:HN39	1.59	0.67
1:E:18:MET:HB2	1:E:29:ILE:HD13	1.76	0.67
1:B:198:TYR:OH	2:B:394:PB0:H32	1.96	0.66
1:E:63:LEU:HG	1:E:81:GLY:HA2	1.77	0.66
1:E:234:LEU:HD13	1:E:337:ILE:HG12	1.78	0.65
1:D:128:ARG:HG3	1:D:128:ARG:NH1	2.09	0.65
1:E:32:ASP:OD2	1:E:35:SER:OG	2.13	0.65
1:A:163:GLN:HA	1:A:166:VAL:CG1	2.27	0.65
1:D:314:THR:HG22	1:D:314:THR:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:ASP:OD1	1:D:312:VAL:HG23	1.98	0.64
1:D:311:ASP:OD1	1:D:312:VAL:HG22	1.97	0.63
1:E:301:LEU:HB3	1:E:302:PRO:HD2	1.81	0.63
1:D:311:ASP:HB3	1:D:314:THR:HA	1.82	0.61
1:D:59:THR:HG23	1:D:83:ASP:OD1	2.01	0.61
1:A:163:GLN:HA	1:A:166:VAL:HG12	1.82	0.61
1:E:297:ARG:NH2	1:E:371:GLU:OE1	2.33	0.60
1:B:10:SER:HB3	1:B:339:GLU:OE2	2.02	0.59
1:A:251:ALA:HB3	1:A:281:PRO:HG3	1.84	0.59
1:B:110:ILE:CD1	2:B:394:PB0:H26A	2.32	0.59
1:D:234:LEU:HD13	1:D:337:ILE:HG13	1.85	0.59
1:A:379:MET:O	1:A:381:ASP:N	2.35	0.59
1:E:110:ILE:HD11	2:E:394:PB0:C26	2.32	0.59
1:D:77:GLU:HB3	1:D:104:GLU:HB2	1.85	0.59
1:E:199:TYR:HB3	1:E:352:ILE:HD11	1.84	0.58
1:E:37:ASN:HB2	3:E:400:HOH:O	2.03	0.58
1:E:251:ALA:HB3	1:E:281:PRO:HG3	1.85	0.58
1:D:295:SER:HB3	1:D:379:MET:HE2	1.84	0.58
1:D:144:THR:HG23	1:D:146:VAL:H	1.68	0.58
1:E:48:LEU:H	1:E:48:LEU:HD12	1.69	0.58
1:D:238:LYS:O	1:D:242:GLU:CG	2.51	0.57
1:D:2:MET:HE2	1:D:176:ILE:H	1.69	0.57
1:E:19:THR:OG1	1:E:86:SER:HB2	2.04	0.57
1:E:174:MET:HE3	1:E:176:ILE:HD11	1.86	0.57
1:E:130:ASP:OD1	1:E:132:SER:HB3	2.04	0.57
1:A:162:ASN:OD1	1:A:165:GLU:OE1	2.23	0.57
1:E:110:ILE:HD11	2:E:394:PB0:H26A	1.86	0.57
1:B:65:LYS:HB3	1:B:80:LEU:HD12	1.88	0.56
1:D:379:MET:HA	1:D:382:CYS:SG	2.46	0.56
1:E:110:ILE:CD1	2:E:394:PB0:C26	2.84	0.55
1:A:241:PHE:CE2	1:A:326:GLN:HG2	2.41	0.55
1:B:376:THR:OG1	1:B:379:MET:HE2	2.07	0.54
1:D:52:TYR:CE2	1:D:54:ARG:HG2	2.43	0.54
1:E:174:MET:HE2	1:E:176:ILE:HD11	1.89	0.54
1:B:218:LYS:HD2	1:B:381:ASP:O	2.08	0.54
1:E:2:MET:CE	1:E:176:ILE:H	2.18	0.54
1:D:28:ASN:HB2	1:D:115:TRP:HA	1.89	0.54
1:D:212:ASP:H	1:E:278:ASN:HD21	1.55	0.54
1:E:226:ILE:HD12	1:E:228:ASP:HB2	1.90	0.54
1:A:153:GLN:HG2	1:A:155:CYS:SG	2.48	0.54
1:D:292:THR:O	1:D:293:ASN:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LEU:O	1:D:144:THR:CG2	2.46	0.53
1:D:202:ILE:CG2	1:D:382:CYS:HB2	2.39	0.53
1:E:163:GLN:C	1:E:167:LEU:HD12	2.22	0.53
2:B:394:PB0:H19A	3:B:437:HOH:O	2.08	0.53
1:D:97:ALA:O	1:D:99:ILE:HD12	2.09	0.53
1:D:2:MET:CE	1:D:90:GLY:HA2	2.39	0.53
1:E:367:THR:HG23	1:E:368:ALA:O	2.08	0.53
1:A:225:SER:OG	1:A:331:THR:HB	2.09	0.53
1:E:376:THR:HB	1:E:379:MET:HE2	1.91	0.53
1:D:218:LYS:HG3	1:D:381:ASP:O	2.09	0.52
1:D:312:VAL:HG23	1:D:313:ALA:H	1.73	0.52
1:E:336:VAL:HG23	1:E:337:ILE:HD12	1.91	0.52
1:B:234:LEU:HD22	1:B:337:ILE:HD11	1.91	0.52
1:D:315:SER:OG	1:D:316:GLN:N	2.41	0.52
1:B:245:VAL:HG12	1:B:249:LYS:HE3	1.91	0.52
1:B:19:THR:OG1	1:B:86:SER:HB2	2.09	0.52
1:B:267:LEU:HD13	1:B:269:CYS:SG	2.49	0.52
1:B:131:ASP:O	1:B:132:SER:HB2	2.06	0.51
1:D:7:ARG:NH1	1:D:167:LEU:HD23	2.24	0.51
1:E:300:ILE:HD13	1:E:337:ILE:HG13	1.91	0.51
1:A:295:SER:HB3	1:A:379:MET:HE2	1.92	0.51
1:B:298:ILE:HG22	1:B:370:VAL:HG22	1.91	0.51
1:E:30:LEU:HD23	1:E:118:ILE:HD12	1.93	0.51
1:A:26:THR:HG22	1:A:50:ARG:NH1	2.26	0.50
1:B:313:ALA:O	1:B:314:THR:HG22	2.11	0.50
1:D:128:ARG:CG	1:D:128:ARG:NH1	2.53	0.50
1:E:281:PRO:HD2	1:E:305:TYR:OH	2.10	0.50
1:D:147:PRO:HB2	1:D:149:LEU:HD23	1.94	0.50
1:A:148:ASN:HB3	1:A:348:ALA:HB2	1.94	0.50
1:E:269:CYS:CB	1:E:319:CYS:HG	2.21	0.50
1:D:202:ILE:HG21	1:D:382:CYS:HB2	1.93	0.50
1:B:47:PHE:CE1	1:B:111:ASN:HB2	2.47	0.49
1:D:364:GLU:OE2	1:E:374:PHE:HB3	2.11	0.49
1:E:313:ALA:O	1:E:314:THR:HG22	2.12	0.49
1:A:2:MET:HG2	1:A:175:ILE:HA	1.95	0.49
1:A:376:THR:O	1:A:379:MET:HE3	2.13	0.49
1:E:149:LEU:HD12	1:E:346:ASP:HA	1.94	0.49
1:D:188:LEU:HD13	1:D:355:ALA:HB2	1.95	0.49
1:B:71:TYR:CG	2:B:394:PB0:H6	2.48	0.48
1:D:3:VAL:O	1:D:4:ASP:HB2	2.13	0.48
1:A:352:ILE:HG22	1:A:354:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:TYR:CD1	1:A:28:ASN:HB3	2.49	0.48
1:D:314:THR:O	1:D:314:THR:CG2	2.61	0.48
1:E:286:TYR:CZ	1:E:297:ARG:HD3	2.48	0.48
1:A:357:SER:HB3	1:A:360:HIS:HB3	1.96	0.48
1:D:207:GLU:HB2	1:D:284:SER:HB2	1.96	0.48
1:E:14:TYR:CD2	1:E:154:LEU:HG	2.49	0.48
1:E:95:VAL:HG21	1:E:140:LEU:HA	1.95	0.48
1:B:300:ILE:HD13	1:B:337:ILE:HD13	1.95	0.48
1:B:334:GLY:O	1:B:338:MET:HG3	2.14	0.48
1:D:48:LEU:HD21	1:D:109:PHE:CD1	2.49	0.47
1:A:28:ASN:HB2	1:A:115:TRP:HA	1.95	0.47
1:D:148:ASN:HB3	1:D:348:ALA:HB2	1.96	0.47
1:D:311:ASP:OD1	1:D:312:VAL:N	2.47	0.47
1:B:14:TYR:CD2	1:B:154:LEU:HG	2.50	0.47
1:D:259:ASP:N	1:D:259:ASP:OD1	2.48	0.47
1:D:376:THR:O	1:D:379:MET:HE3	2.14	0.47
1:D:30:LEU:HD23	1:D:118:ILE:HD12	1.96	0.47
1:B:376:THR:O	1:B:379:MET:HE2	2.15	0.47
1:E:130:ASP:OD1	1:E:132:SER:CB	2.63	0.47
1:E:357:SER:HB3	1:E:360:HIS:HB3	1.97	0.46
1:D:45:HIS:CG	1:D:46:PRO:HD2	2.51	0.46
1:E:20:VAL:O	1:E:25:GLN:HG3	2.15	0.46
1:E:295:SER:HB3	1:E:379:MET:HE1	1.98	0.46
1:E:337:ILE:HD12	1:E:337:ILE:N	2.31	0.46
1:E:48:LEU:H	1:E:48:LEU:CD1	2.29	0.46
1:E:364:GLU:OE1	1:E:364:GLU:N	2.46	0.45
1:E:363:ASP:OD1	1:E:363:ASP:N	2.49	0.45
1:D:151:SER:HB2	1:D:342:TYR:CE1	2.52	0.45
1:D:311:ASP:HB3	1:D:314:THR:CA	2.45	0.45
1:E:309:VAL:HG11	1:E:321:LYS:HD2	1.98	0.45
1:B:53:GLN:HB3	1:B:56:LEU:HD13	1.98	0.45
1:B:18:MET:HG2	1:B:87:ILE:HG12	1.98	0.45
1:E:251:ALA:CB	1:E:281:PRO:HG3	2.47	0.45
1:E:336:VAL:HG23	1:E:337:ILE:CD1	2.46	0.45
1:D:341:PHE:HB3	1:D:355:ALA:O	2.17	0.45
1:E:113:SER:HB2	1:E:115:TRP:NE1	2.31	0.45
1:D:51:TYR:CD2	1:D:51:TYR:N	2.85	0.45
1:E:63:LEU:HD12	1:E:80:LEU:HB3	1.97	0.44
1:E:71:TYR:CG	2:E:394:PB0:H6	2.51	0.44
1:E:311:ASP:OD1	1:E:312:VAL:N	2.50	0.44
1:D:235:ARG:HB3	1:D:327:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ILE:HB	1:D:341:PHE:CZ	2.52	0.44
1:B:310:GLU:OE1	1:B:310:GLU:HA	2.18	0.44
1:B:238:LYS:HG3	1:B:326:GLN:HE21	1.83	0.44
1:A:223:ASP:OD2	1:A:224:LYS:NZ	2.48	0.44
1:B:131:ASP:OD1	1:B:131:ASP:C	2.55	0.44
1:A:22:SER:O	1:A:57:SER:HA	2.19	0.43
1:B:298:ILE:HB	1:B:341:PHE:CZ	2.52	0.43
1:D:91:PRO:HB2	1:D:93:VAL:HG22	2.00	0.43
1:D:305:TYR:HB2	1:D:324:ILE:HD12	2.00	0.43
1:B:130:ASP:OD1	1:B:132:SER:CB	2.56	0.43
1:D:2:MET:HE1	1:D:91:PRO:HD3	2.00	0.43
1:A:304:GLN:O	1:A:336:VAL:HB	2.18	0.43
1:B:205:ARG:HB3	1:B:286:TYR:CG	2.54	0.43
1:B:360:HIS:HA	3:B:421:HOH:O	2.17	0.43
1:D:18:MET:SD	1:D:29:ILE:HG13	2.59	0.43
1:D:197:TRP:CG	1:D:198:TYR:N	2.85	0.43
1:D:305:TYR:HB2	1:D:324:ILE:CD1	2.49	0.43
1:E:36:SER:OG	1:E:126:ILE:HG13	2.18	0.43
1:E:346:ASP:HB3	1:E:351:ARG:HG3	2.01	0.43
1:D:146:VAL:HG11	1:D:176:ILE:HG22	2.00	0.43
1:B:15:TYR:CD1	1:B:28:ASN:HB3	2.54	0.42
1:B:110:ILE:HD11	2:B:394:PB0:H26A	2.00	0.42
1:D:47:PHE:CE1	1:D:111:ASN:HB2	2.54	0.42
1:D:225:SER:OG	1:D:331:THR:HB	2.19	0.42
1:A:378:ASP:O	1:A:379:MET:CB	2.51	0.42
1:B:45:HIS:CG	1:B:46:PRO:HD2	2.54	0.42
1:E:67:VAL:HG13	1:E:76:TRP:HZ3	1.85	0.42
1:A:123:TYR:CZ	1:A:196:GLU:HG2	2.55	0.42
1:B:234:LEU:HB2	1:B:337:ILE:HD11	2.00	0.42
1:D:212:ASP:H	1:E:278:ASN:ND2	2.17	0.42
1:D:128:ARG:HH11	1:D:128:ARG:HG2	1.77	0.42
1:A:234:LEU:HD23	1:A:324:ILE:HG12	2.01	0.42
1:E:137:PHE:HE1	1:E:176:ILE:CD1	2.33	0.42
1:B:3:VAL:O	1:B:4:ASP:HB2	2.20	0.42
1:A:314:THR:HG22	1:A:314:THR:O	2.20	0.41
1:B:245:VAL:CG1	1:B:249:LYS:HE3	2.50	0.41
1:A:181:HIS:HA	1:A:184:TYR:CE2	2.55	0.41
1:D:208:ILE:HG13	1:D:247:SER:HB3	2.02	0.41
1:A:315:SER:OG	1:A:316:GLN:N	2.53	0.41
1:D:160:PRO:HB3	1:D:310:GLU:OE1	2.19	0.41
1:D:195:ARG:HB3	1:D:197:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD23	1:B:118:ILE:HD12	2.03	0.41
2:B:394:PB0:H26	2:B:394:PB0:HN39	1.86	0.41
1:D:234:LEU:HB2	1:D:337:ILE:CD1	2.33	0.41
1:B:55:GLN:CG	1:B:56:LEU:HD12	2.51	0.41
1:E:110:ILE:CD1	2:E:394:PB0:H26A	2.49	0.41
1:E:134:GLU:HA	1:E:135:PRO:HD3	1.96	0.41
1:E:216:ASP:OD2	1:E:218:LYS:HB2	2.21	0.41
1:E:364:GLU:H	1:E:364:GLU:CD	2.22	0.41
1:A:41:GLY:O	1:A:51:TYR:HB2	2.20	0.41
1:A:291:VAL:O	1:A:294:GLN:HB3	2.20	0.41
1:B:153:GLN:HG2	1:B:183:LEU:HD13	2.03	0.40
1:D:379:MET:CA	1:D:382:CYS:SG	3.09	0.40
1:E:71:TYR:CB	2:E:394:PB0:H6	2.52	0.40
1:E:18:MET:HB2	1:E:29:ILE:CD1	2.48	0.40
1:E:107:LYS:HZ3	1:E:107:LYS:HG2	1.78	0.40
1:B:376:THR:OG1	1:B:379:MET:CE	2.70	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ALA:O	1:D:312:VAL:CG1[2_646]	1.34	0.86
1:A:313:ALA:C	1:D:312:VAL:CG1[2_646]	2.02	0.18
1:A:313:ALA:CB	1:D:312:VAL:N[2_646]	2.03	0.17
1:B:75:LYS:NZ	1:E:106:ASP:OD1[2_656]	2.04	0.16
1:A:313:ALA:CB	1:D:312:VAL:CA[2_646]	2.06	0.14
1:B:106:ASP:OD1	1:E:107:LYS:CE[2_656]	2.18	0.02
1:B:106:ASP:OD1	1:E:107:LYS:NZ[2_656]	2.19	0.01

## 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	384/455 (84%)	372 (97%)	11 (3%)	1 (0%)	37	54
1	B	384/455 (84%)	372 (97%)	10 (3%)	2 (0%)	25	42
1	D	384/455 (84%)	369 (96%)	13 (3%)	2 (0%)	25	42
1	E	384/455 (84%)	373 (97%)	9 (2%)	2 (0%)	25	42
All	All	1536/1820 (84%)	1486 (97%)	43 (3%)	7 (0%)	25	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	GLU
1	B	132	SER
1	B	380	GLU
1	E	380	GLU
1	D	378	ASP
1	E	223	ASP
1	D	223	ASP

### 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%)	313 (95%)	16 (5%)	21	40
1	B	329/381 (86%)	316 (96%)	13 (4%)	27	48
1	D	329/381 (86%)	313 (95%)	16 (5%)	21	40
1	E	329/381 (86%)	316 (96%)	13 (4%)	27	48
All	All	1316/1524 (86%)	1258 (96%)	58 (4%)	24	44

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

Mol	Chain	Res	Type
1	A	0	VAL
1	A	26	THR
1	A	149	LEU
1	A	162	ASN

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Mol	Chain	Res	Type
1	A	169	SER
1	A	170	VAL
1	A	185	THR
1	A	197	TRP
1	A	239	LYS
1	A	245	VAL
1	A	253	SER
1	A	263	LEU
1	A	265	GLU
1	A	279	ILE
1	A	316	GLN
1	A	359	CYS
1	B	55	GLN
1	B	65	LYS
1	B	77	GLU
1	B	104	GLU
1	B	105	SER
1	B	131	ASP
1	B	154	LEU
1	B	162	ASN
1	B	197	TRP
1	B	218	LYS
1	B	239	LYS
1	B	314	THR
1	B	316	GLN
1	D	55	GLN
1	D	65	LYS
1	D	88	PRO
1	D	94	THR
1	D	128	ARG
1	D	130	ASP
1	D	188	LEU
1	D	197	TRP
1	D	247	SER
1	D	259	ASP
1	D	263	LEU
1	D	292	THR
1	D	312	VAL
1	D	367	THR
1	D	377	LEU
1	D	382	CYS
1	E	38	PHE

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Mol	Chain	Res	Type
1	E	55	GLN
1	E	85	VAL
1	E	105	SER
1	E	107	LYS
1	E	149	LEU
1	E	169	SER
1	E	182	SER
1	E	197	TRP
1	E	364	GLU
1	E	367	THR
1	E	377	LEU
1	E	381	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	111	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](#)

4 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	PB0	D	394	-	50,50,50	0.79	1 (2%)	56,70,70	1.91	12 (21%)
2	PB0	B	394	-	50,50,50	0.59	0	56,70,70	1.90	13 (23%)
2	PB0	E	394	-	50,50,50	0.66	0	56,70,70	2.00	13 (23%)
2	PB0	A	394	-	50,50,50	0.72	1 (2%)	56,70,70	1.70	13 (23%)

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	PB0	D	394	-	-	10/43/68/68	0/4/4/4
2	PB0	B	394	-	-	8/43/68/68	0/4/4/4
2	PB0	E	394	-	-	6/43/68/68	0/4/4/4
2	PB0	A	394	-	-	7/43/68/68	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	394	PB0	C22-C13	-2.99	1.50	1.52
2	A	394	PB0	C22-C13	-2.11	1.50	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	394	PB0	C18-N38-C13	-7.77	108.52	113.47
2	B	394	PB0	C18-N38-C13	-6.90	109.07	113.47
2	D	394	PB0	O41-C13-C22	-5.63	121.79	126.75
2	A	394	PB0	C18-N38-C13	-5.45	109.99	113.47
2	D	394	PB0	C18-N38-C13	-5.30	110.09	113.47
2	E	394	PB0	O41-C13-C22	-4.50	122.79	126.75
2	D	394	PB0	C29-C22-N39	4.50	118.46	108.96
2	D	394	PB0	C16-C18-N38	4.21	107.69	103.19
2	B	394	PB0	O42-C14-C23	-4.01	114.92	122.05
2	E	394	PB0	O42-C14-C23	-3.90	115.11	122.05
2	B	394	PB0	C22-N39-C14	3.77	128.29	122.98
2	A	394	PB0	C29-C22-N39	3.65	116.67	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	394	PB0	C8-C12-C7	-3.61	119.12	123.50
2	B	394	PB0	C33-N38-C13	3.45	126.24	122.12
2	E	394	PB0	C23-C14-N39	3.44	120.22	115.94
2	E	394	PB0	C33-N38-C13	3.30	126.07	122.12
2	E	394	PB0	C10-C7-C12	3.28	121.61	118.75
2	B	394	PB0	C29-C22-N39	3.24	115.80	108.96
2	A	394	PB0	C10-C6-C11	3.17	121.51	118.75
2	B	394	PB0	C16-C18-N38	3.13	106.53	103.19
2	A	394	PB0	O42-C14-C23	-3.09	116.56	122.05
2	B	394	PB0	O41-C13-C22	-3.08	124.04	126.75
2	E	394	PB0	C16-C18-N38	3.06	106.46	103.19
2	A	394	PB0	C16-C18-N38	3.06	106.45	103.19
2	E	394	PB0	C29-C22-N39	3.04	115.38	108.96
2	D	394	PB0	C10-C6-C11	3.02	121.38	118.75
2	A	394	PB0	C33-N38-C13	2.99	125.70	122.12
2	B	394	PB0	O43-C15-N40	-2.99	117.60	122.96
2	E	394	PB0	C22-N39-C14	2.93	127.10	122.98
2	B	394	PB0	C8-C12-C7	-2.85	120.03	123.50
2	D	394	PB0	O42-C14-C23	-2.78	117.10	122.05
2	D	394	PB0	C31-C27-C9	-2.75	104.17	113.22
2	A	394	PB0	C22-N39-C14	2.73	126.82	122.98
2	B	394	PB0	C22-C29-C35	2.65	122.97	118.27
2	B	394	PB0	C23-C14-N39	2.64	119.22	115.94
2	B	394	PB0	O42-C14-N39	2.62	125.86	122.23
2	D	394	PB0	C28-C36-N40	-2.62	106.36	110.08
2	D	394	PB0	C33-N38-C13	2.56	125.18	122.12
2	A	394	PB0	C10-C7-C12	2.49	120.92	118.75
2	D	394	PB0	C20-C17-C21	2.43	107.13	102.24
2	A	394	PB0	C8-C12-C7	-2.42	120.57	123.50
2	D	394	PB0	C8-C11-C6	-2.36	120.63	123.50
2	A	394	PB0	C20-C17-C21	2.33	106.94	102.24
2	A	394	PB0	C17-C20-C19	-2.28	101.72	103.68
2	A	394	PB0	C23-C14-N39	2.27	118.77	115.94
2	E	394	PB0	C12-C8-C11	2.13	119.19	116.08
2	E	394	PB0	F47-C12-C8	2.12	121.29	118.28
2	D	394	PB0	C22-N39-C14	2.10	125.94	122.98
2	E	394	PB0	C22-C29-C35	2.09	121.98	118.27
2	A	394	PB0	C8-C11-C6	-2.02	121.04	123.50
2	B	394	PB0	C8-C11-C6	-2.00	121.07	123.50

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	394	PB0	C17-C20-O45-C32
2	A	394	PB0	C13-C22-C29-C35
2	A	394	PB0	C16-C22-C29-C35
2	A	394	PB0	N39-C22-C29-C35
2	B	394	PB0	C17-C20-O45-C32
2	B	394	PB0	C13-C22-C29-C35
2	B	394	PB0	C16-C22-C29-C35
2	B	394	PB0	N39-C22-C29-C35
2	B	394	PB0	C30-C32-O45-C20
2	D	394	PB0	C13-C22-C29-C35
2	D	394	PB0	C16-C22-C29-C35
2	D	394	PB0	N39-C22-C29-C35
2	D	394	PB0	C27-C31-C33-N38
2	E	394	PB0	C13-C22-C29-C35
2	E	394	PB0	C16-C22-C29-C35
2	E	394	PB0	N39-C22-C29-C35
2	E	394	PB0	C31-C33-N38-C18
2	E	394	PB0	O44-C34-C36-N40
2	E	394	PB0	C15-C33-N38-C18
2	B	394	PB0	C19-C20-O45-C32
2	D	394	PB0	C24-C30-C32-O45
2	B	394	PB0	C31-C33-N38-C18
2	D	394	PB0	C27-C31-C33-C15
2	A	394	PB0	C19-C20-O45-C32
2	D	394	PB0	C13-C22-N39-C14
2	D	394	PB0	C31-C33-N38-C18
2	D	394	PB0	C6-C10-C28-C36
2	A	394	PB0	C6-C10-C28-C36
2	B	394	PB0	C15-C33-N38-C18
2	D	394	PB0	C7-C10-C28-C36
2	A	394	PB0	C7-C10-C28-C36

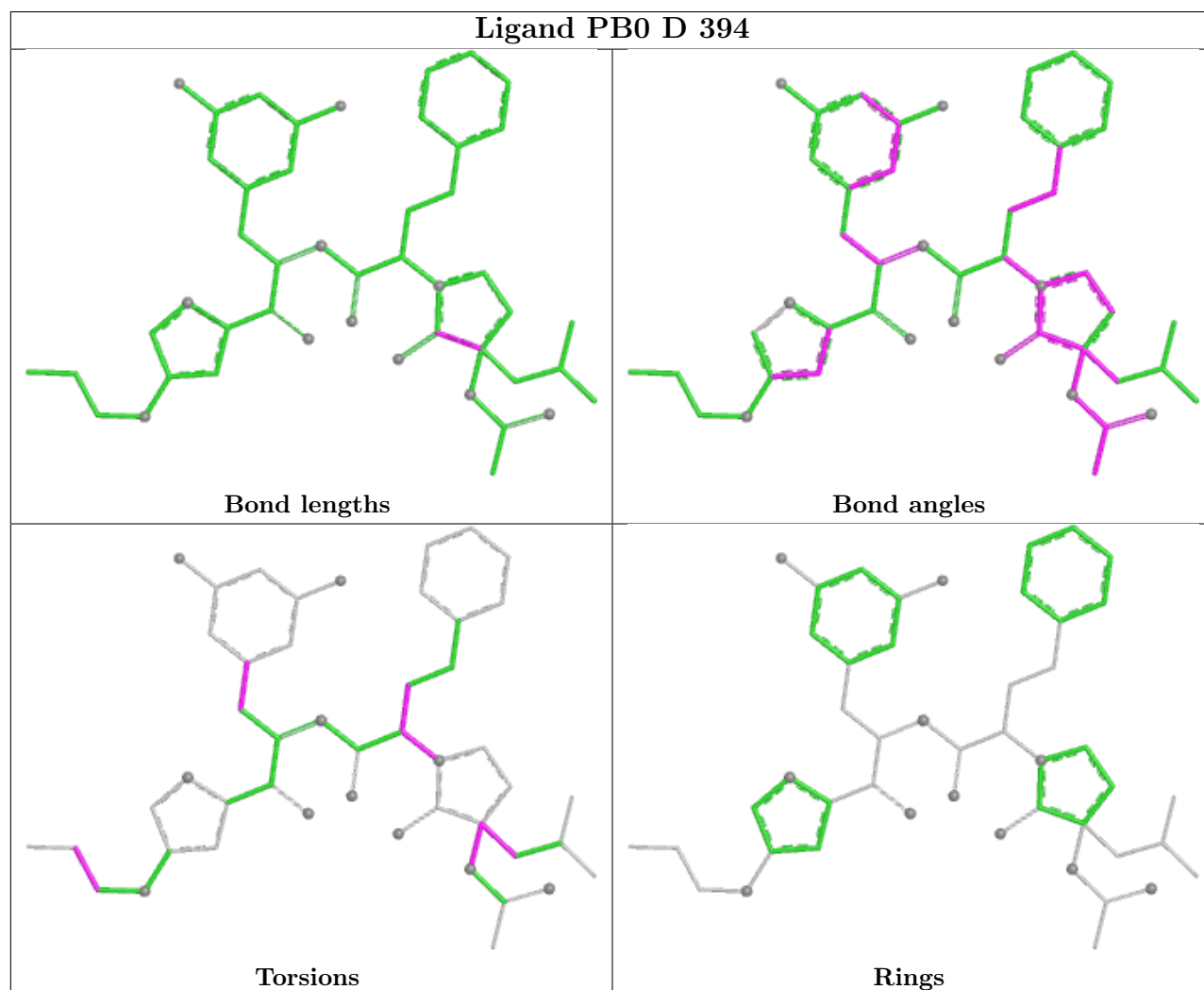
There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	394	PB0	1	0
2	B	394	PB0	6	0
2	E	394	PB0	6	0

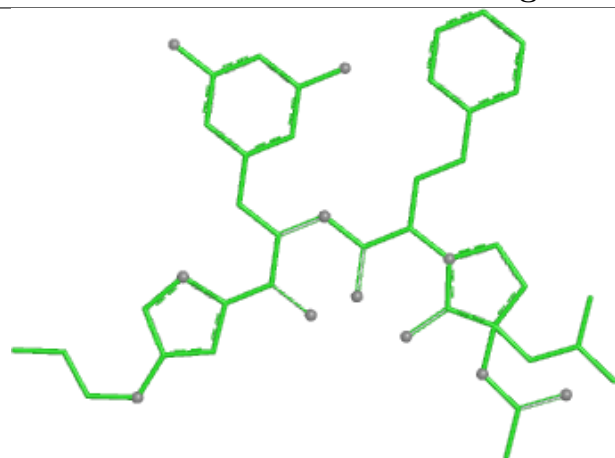
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

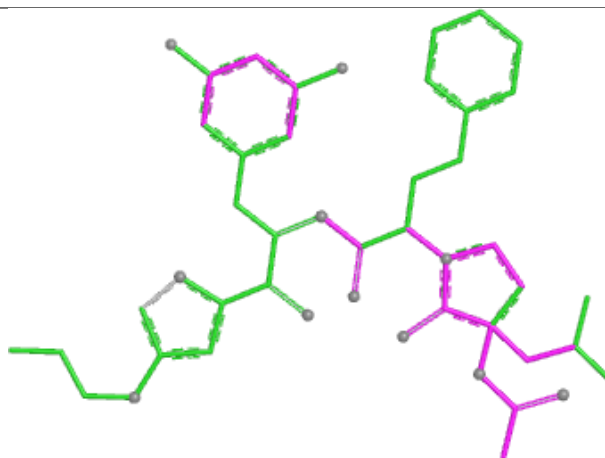




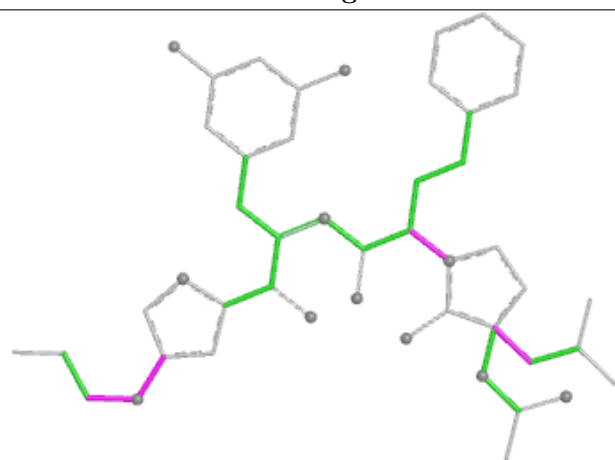
## Ligand PB0 B 394



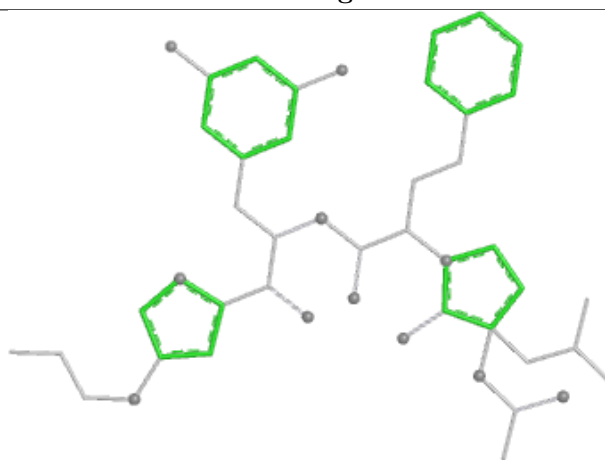
Bond lengths



Bond angles

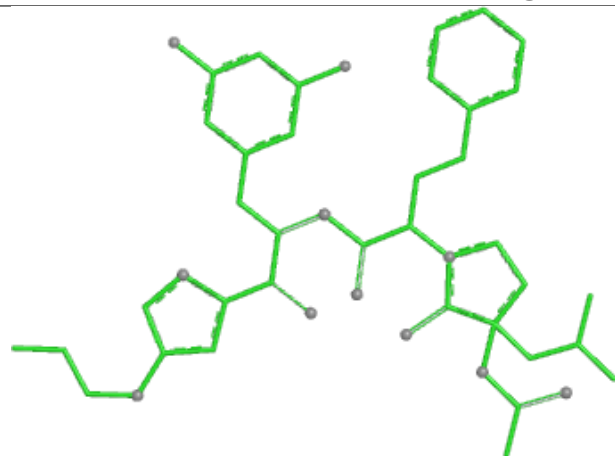


Torsions

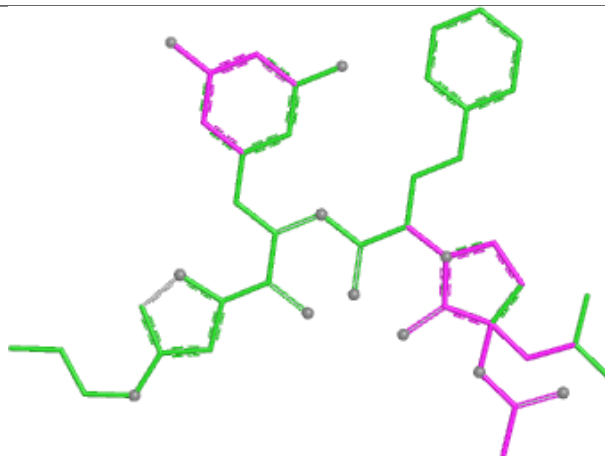


Rings

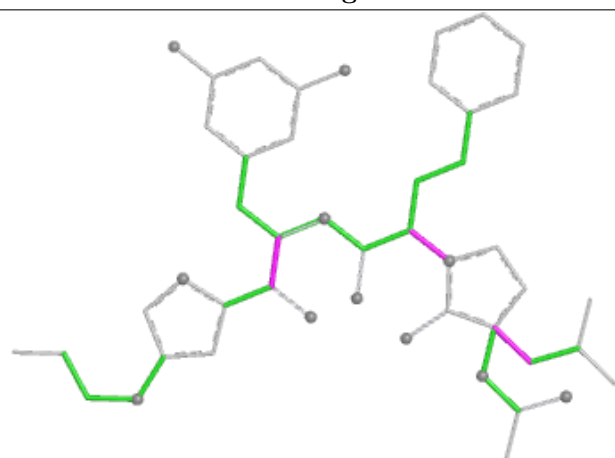
## Ligand PB0 E 394



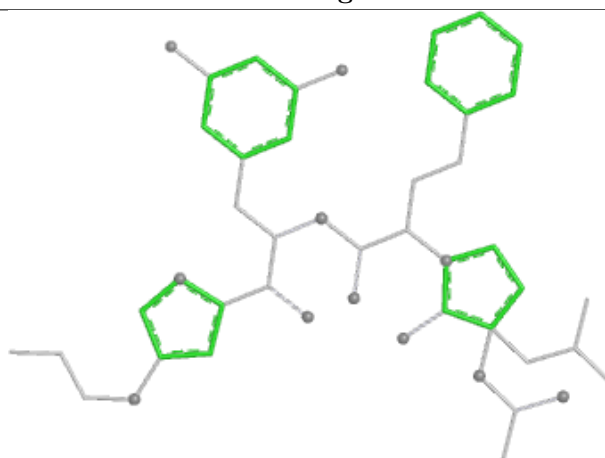
Bond lengths



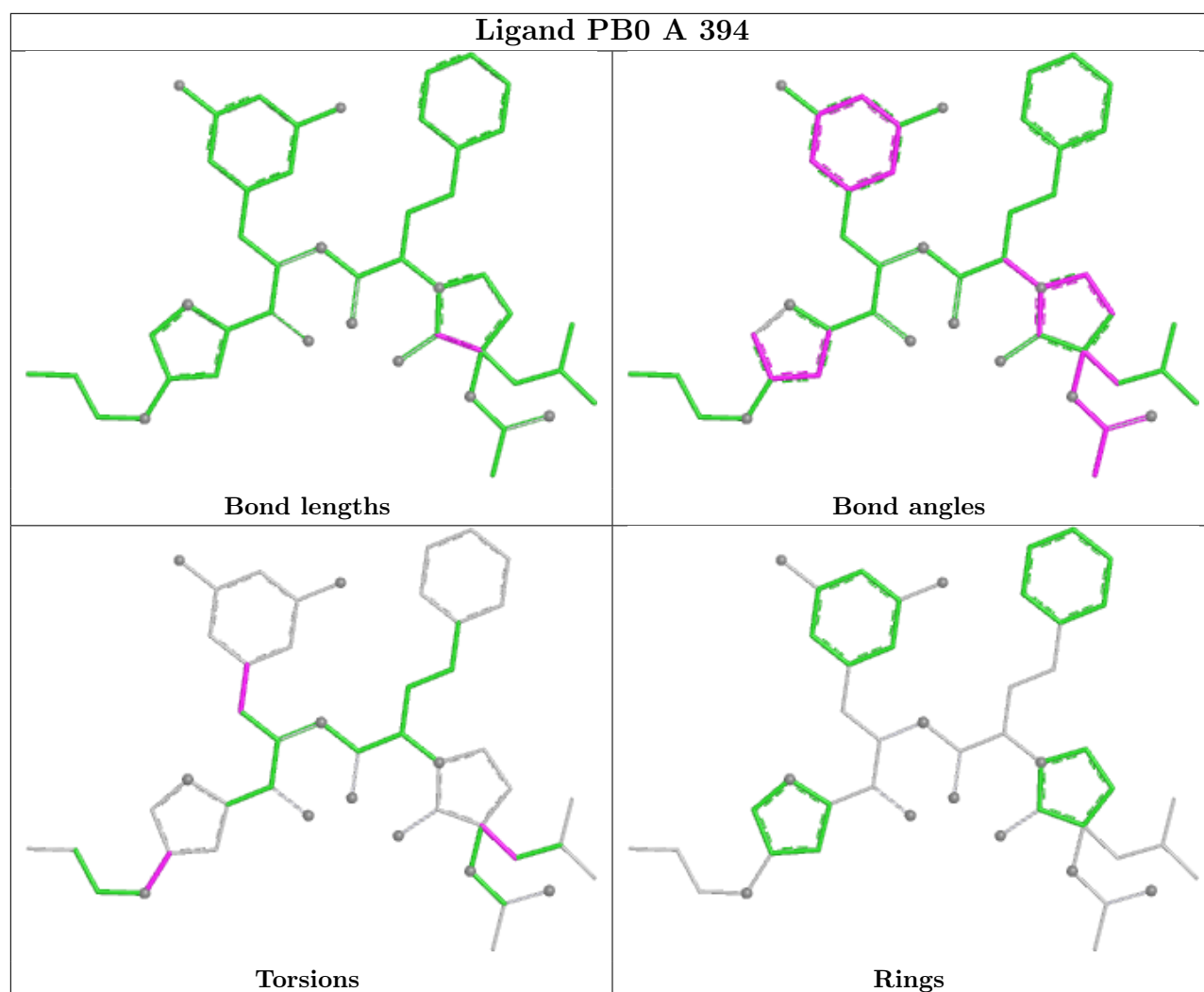
Bond angles



Torsions



Rings



## 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	386/455 (84%)	0.71	29 (7%)	22	21	12, 22, 34, 44	0
1	B	386/455 (84%)	0.71	27 (6%)	24	23	12, 22, 34, 44	0
1	D	386/455 (84%)	0.81	32 (8%)	19	19	13, 22, 34, 44	0
1	E	386/455 (84%)	0.78	26 (6%)	25	24	13, 22, 34, 44	0
All	All	1544/1820 (84%)	0.75	114 (7%)	22	21	12, 22, 34, 44	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	THR	7.3
1	A	376	THR	7.3
1	B	314	THR	6.5
1	A	378	ASP	6.2
1	B	378	ASP	5.3
1	B	313	ALA	5.3
1	E	377	LEU	5.2
1	A	377	LEU	4.9
1	E	313	ALA	4.7
1	B	312	VAL	4.5
1	D	311	ASP	4.4
1	D	312	VAL	4.3
1	D	145	HIS	4.2
1	B	380	GLU	4.2
1	D	377	LEU	4.2
1	E	376	THR	4.1
1	E	378	ASP	4.1
1	D	313	ALA	4.1
1	A	381	ASP	4.1
1	A	380	GLU	4.0
1	A	375	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	315	SER	4.0
1	B	377	LEU	3.9
1	B	0	VAL	3.9
1	B	384	TYR	3.9
1	D	375	VAL	3.9
1	D	376	THR	3.8
1	D	384	TYR	3.7
1	B	379	MET	3.7
1	E	312	VAL	3.6
1	D	380	GLU	3.5
1	D	378	ASP	3.5
1	E	314	THR	3.5
1	E	168	ALA	3.4
1	B	292	THR	3.3
1	A	315	SER	3.3
1	B	293	ASN	3.2
1	D	43	ALA	3.2
1	E	380	GLU	3.2
1	D	383	GLY	3.2
1	D	315	SER	3.1
1	A	292	THR	3.1
1	A	312	VAL	3.0
1	E	3	VAL	3.0
1	D	49	HIS	3.0
1	E	169	SER	3.0
1	B	162	ASN	3.0
1	A	291	VAL	2.9
1	E	43	ALA	2.9
1	E	311	ASP	2.9
1	A	379	MET	2.8
1	E	379	MET	2.8
1	D	258	PRO	2.8
1	A	384	TYR	2.8
1	A	168	ALA	2.7
1	D	141	VAL	2.7
1	A	293	ASN	2.7
1	D	3	VAL	2.6
1	D	218	LYS	2.6
1	E	278	ASN	2.6
1	B	105	SER	2.6
1	E	47	PHE	2.6
1	D	314	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1	GLU	2.5
1	A	311	ASP	2.5
1	A	93	VAL	2.5
1	E	0	VAL	2.5
1	B	169	SER	2.5
1	E	164	SER	2.5
1	D	68	TYR	2.5
1	A	49	HIS	2.4
1	B	139	SER	2.4
1	E	375	VAL	2.4
1	B	7	ARG	2.4
1	A	145	HIS	2.3
1	D	293	ASN	2.3
1	B	364	GLU	2.3
1	D	171	GLY	2.3
1	A	314	THR	2.3
1	D	-1	PHE	2.3
1	D	237	PRO	2.3
1	B	131	ASP	2.3
1	D	1	GLU	2.3
1	A	105	SER	2.3
1	B	-1	PHE	2.3
1	B	223	ASP	2.3
1	A	163	GLN	2.3
1	E	384	TYR	2.3
1	A	313	ALA	2.3
1	A	359	CYS	2.3
1	E	267	LEU	2.2
1	A	171	GLY	2.2
1	D	185	THR	2.2
1	B	44	PRO	2.2
1	A	73	GLN	2.2
1	D	168	ALA	2.2
1	E	49	HIS	2.2
1	B	167	LEU	2.2
1	A	310	GLU	2.2
1	B	242	GLU	2.2
1	D	379	MET	2.1
1	B	112	GLY	2.1
1	E	44	PRO	2.1
1	E	382	CYS	2.1
1	D	267	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	162	ASN	2.1
1	A	181	HIS	2.1
1	D	2	MET	2.1
1	E	-1	PHE	2.1
1	E	23	PRO	2.1
1	D	216	ASP	2.1
1	D	294	GLN	2.0
1	E	105	SER	2.0
1	A	86	SER	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](#)

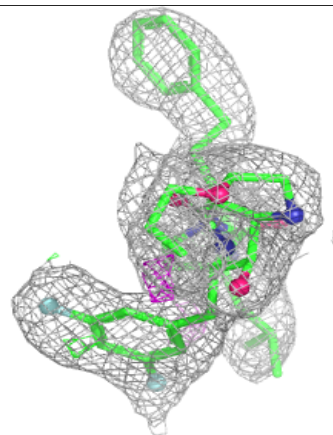
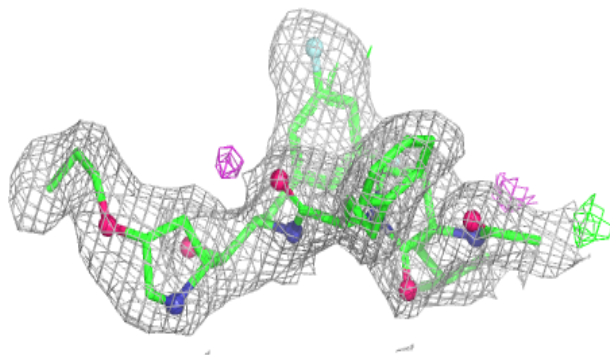
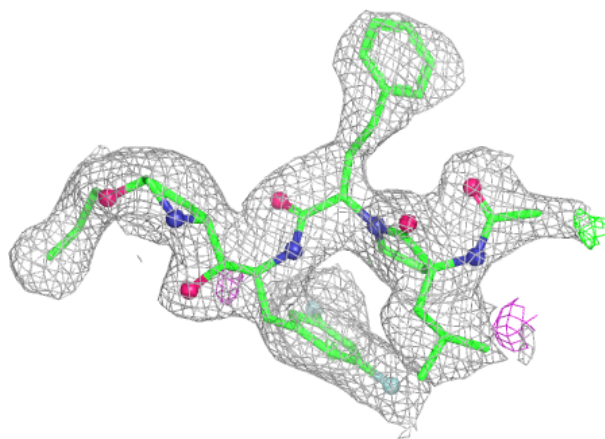
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	PB0	D	394	47/47	0.85	0.14	12,19,22,25	0
2	PB0	A	394	47/47	0.90	0.11	10,18,21,24	0
2	PB0	E	394	47/47	0.90	0.11	13,18,21,24	0
2	PB0	B	394	47/47	0.91	0.11	12,17,20,21	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 PB0 D 394:**

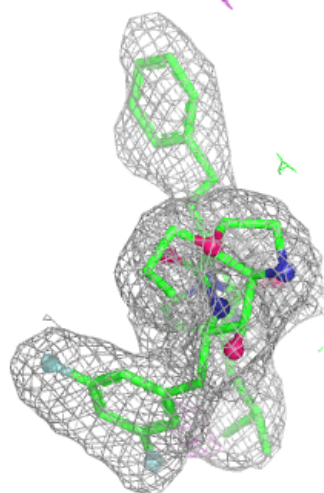
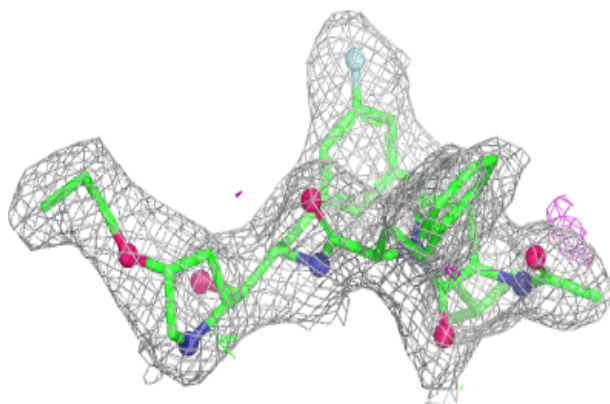
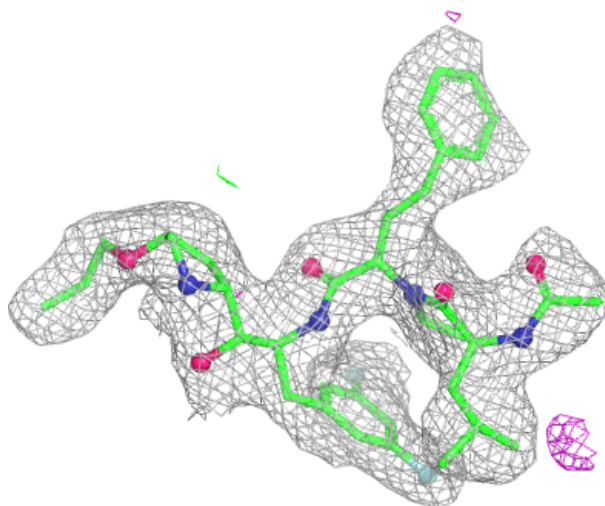
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





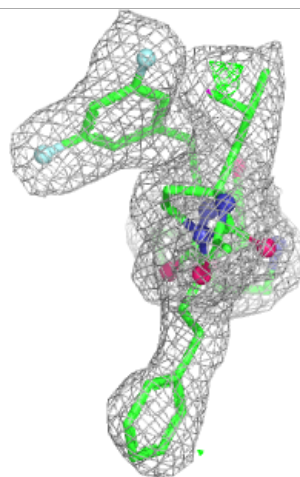
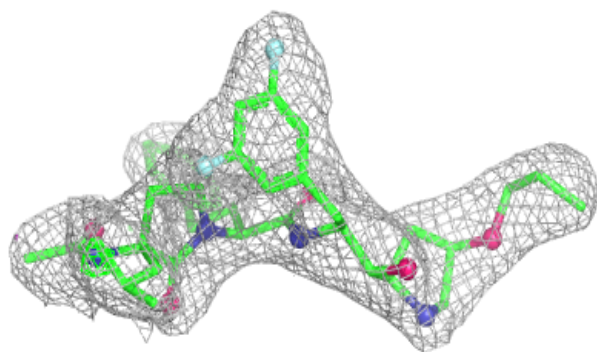
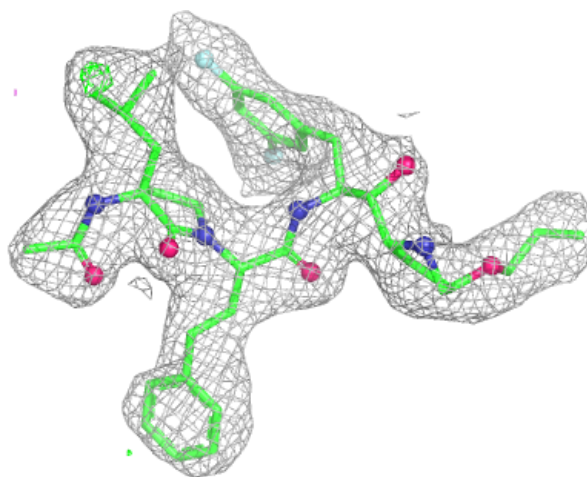
**Electron density around PB0 A 394:**

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



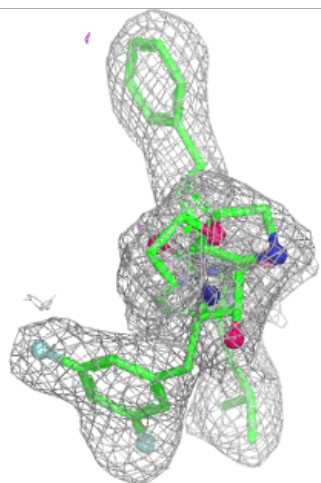
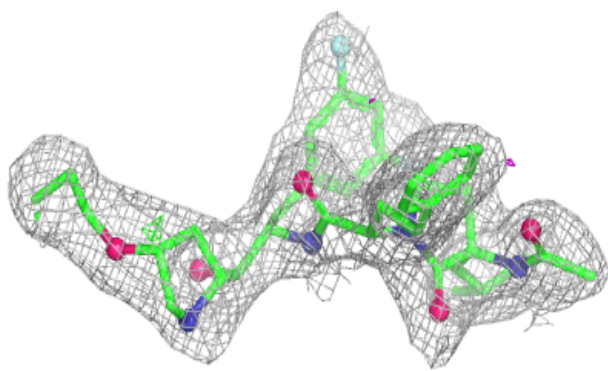
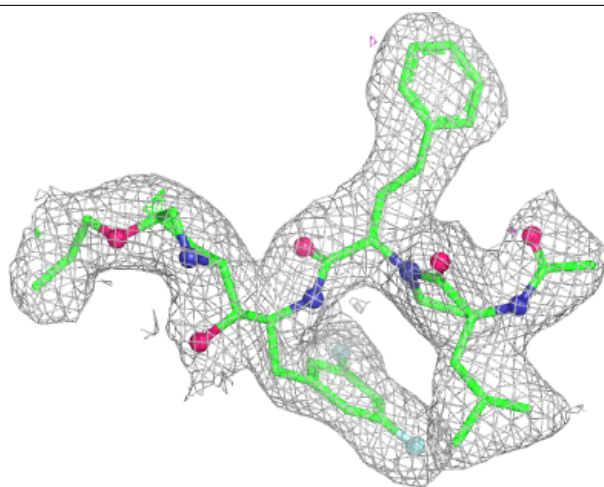
**Electron density around PB0 E 394:**

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



**Electron density around PB0 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.