



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 01:41 AM BST

PDB ID : 3BUM  
Title : Crystal structure of c-Cbl-TKB domain complexed with its binding motif in Sprouty2  
Authors : Ng, C.; Jackson, A.R.; Buschdorf, P.J.; Sun, Q.; Guy, R.G.; Sivaraman, J.  
Deposited on : 2008-01-03  
Resolution : 2.00 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

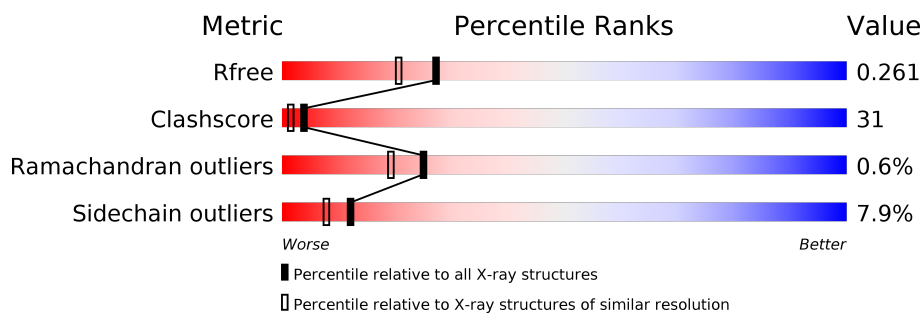
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 on 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	13	
2	B	329	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2860 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 Protein sprouty homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	9	Total	C	N	O	P	0	0	0
			74	42	10	21	1			

- Molecule 2 is a protein called E3 ubiquitin-protein ligase CBL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	304	Total	C	N	O	S	0	0	0
			2489	1612	424	440	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	GLY	-	cloning artifact	UNP P22681
B	24	SER	-	cloning artifact	UNP P22681

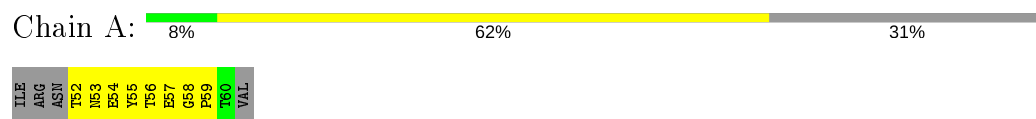
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	283	Total	O	0	0
			283	283		

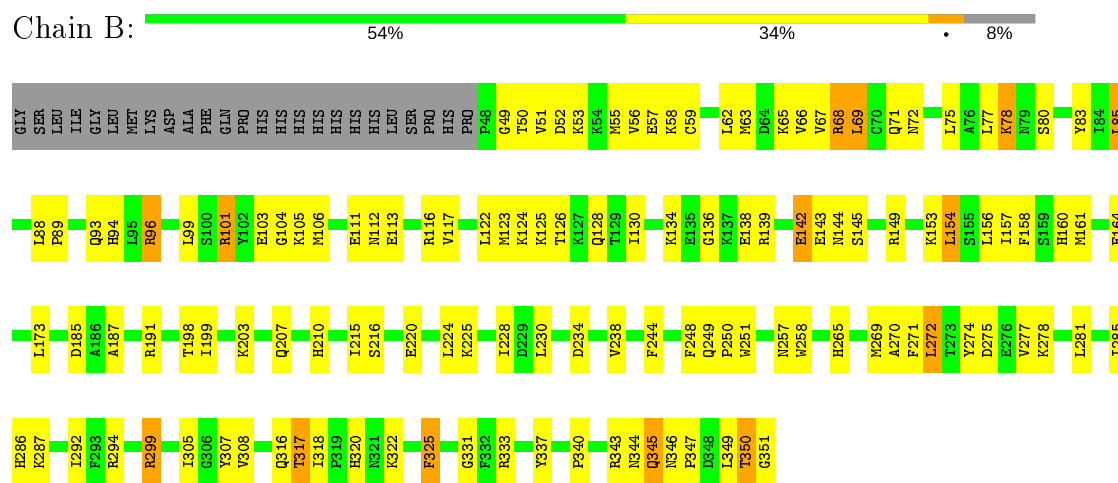
### 3 Residue-property plots

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. 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. 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: Protein sprouty homolog 2



- Molecule 2: E3 ubiquitin-protein ligase CBL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.26 Å   122.26 Å   54.71 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 2.00 48.60 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.00) 99.8 (48.60-1.98)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 1.98 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.263 0.223 , 0.261	Depositor DCC
$R_{free}$ test set	2296 reflections (7.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 31.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.253 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0/57	0.84	0/76
2	B	0.50	0/2555	0.62	0/3449
All	All	0.50	0/2612	0.63	0/3525

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	74	0	55	9	0
2	B	2489	0	2499	155	0
3	A	14	0	0	2	0
3	B	283	0	0	48	0
All	All	2860	0	2554	157	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 31.

All (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ARG:HH12	2:B:316:GLN:HE22	1.05	1.00
2:B:238:VAL:HB	3:B:389:HOH:O	1.62	0.99
2:B:248:PHE:HB3	3:B:511:HOH:O	1.66	0.93
2:B:93:GLN:HE22	2:B:96:ARG:HH11	1.09	0.92
2:B:68:ARG:HH11	2:B:68:ARG:HG2	1.41	0.85
1:A:58:GLY:HA2	2:B:317:THR:HG21	1.59	0.85
2:B:101:ARG:HH11	2:B:101:ARG:HB3	1.42	0.83
2:B:340:PRO:HD3	2:B:346:ASN:HD22	1.44	0.83
2:B:257:ASN:HB2	3:B:511:HOH:O	1.79	0.83
1:A:56:THR:O	2:B:317:THR:HG23	1.79	0.82
2:B:51:VAL:HA	2:B:55:MET:HE3	1.60	0.82
2:B:294:ARG:NH1	2:B:316:GLN:HE22	1.78	0.81
2:B:294:ARG:HH12	2:B:316:GLN:NE2	1.79	0.81
2:B:343:ARG:HD2	3:B:423:HOH:O	1.81	0.81
2:B:347:PRO:HD2	3:B:479:HOH:O	1.81	0.80
2:B:68:ARG:HG3	2:B:69:LEU:N	1.96	0.80
2:B:101:ARG:HH11	2:B:101:ARG:CB	1.93	0.80
2:B:124:LYS:HD2	3:B:433:HOH:O	1.82	0.80
2:B:145:SER:O	2:B:149:ARG:HG2	1.85	0.76
2:B:308:VAL:HG23	3:B:510:HOH:O	1.84	0.76
2:B:277:VAL:HG21	2:B:294:ARG:HH11	1.52	0.75
2:B:220:GLU:HB3	3:B:455:HOH:O	1.87	0.75
2:B:157:ILE:HG12	3:B:497:HOH:O	1.88	0.72
2:B:215:ILE:HG22	3:B:455:HOH:O	1.89	0.72
2:B:210:HIS:HD2	2:B:215:ILE:H	1.37	0.72
2:B:101:ARG:HH11	2:B:101:ARG:CG	2.03	0.71
2:B:51:VAL:HA	2:B:55:MET:CE	2.21	0.71
2:B:75:LEU:HG	3:B:489:HOH:O	1.90	0.70
2:B:53:LYS:O	2:B:57:GLU:HG2	1.92	0.69
2:B:139:ARG:HA	2:B:142:GLU:OE1	1.92	0.69
2:B:113:GLU:O	2:B:117:VAL:HG23	1.92	0.69
2:B:203:LYS:CD	2:B:203:LYS:H	2.06	0.69
2:B:124:LYS:O	2:B:128:GLN:HG3	1.92	0.68
2:B:271:PHE:HB3	3:B:481:HOH:O	1.94	0.68
2:B:333:ARG:HD2	3:B:419:HOH:O	1.92	0.68
2:B:128:GLN:NE2	3:B:496:HOH:O	2.27	0.67
2:B:153:LYS:HA	3:B:481:HOH:O	1.93	0.67
2:B:149:ARG:HH11	2:B:149:ARG:HG3	1.60	0.67
2:B:144:ASN:HA	2:B:149:ARG:HE	1.60	0.67
2:B:228:ILE:HG12	2:B:244:PHE:CD1	2.30	0.66
2:B:203:LYS:HD3	2:B:203:LYS:H	1.61	0.65
2:B:78:LYS:H	2:B:78:LYS:NZ	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:GLN:HE22	2:B:96:ARG:NH1	1.87	0.65
2:B:210:HIS:CD2	2:B:215:ILE:H	2.15	0.65
2:B:346:ASN:ND2	3:B:479:HOH:O	2.29	0.64
2:B:281:LEU:HD13	3:B:510:HOH:O	1.98	0.64
2:B:68:ARG:HG2	2:B:68:ARG:NH1	2.11	0.64
2:B:106:MET:HE2	3:B:438:HOH:O	1.97	0.63
2:B:349:LEU:O	2:B:351:GLY:N	2.30	0.63
1:A:59:PRO:HG3	2:B:307:TYR:CZ	2.34	0.63
2:B:281:LEU:HD22	3:B:510:HOH:O	1.98	0.63
2:B:278:LYS:HD3	3:B:494:HOH:O	1.97	0.63
2:B:75:LEU:N	3:B:489:HOH:O	2.32	0.62
2:B:277:VAL:HG13	2:B:292:ILE:HD11	1.81	0.62
2:B:112:ASN:O	2:B:116:ARG:HG3	1.98	0.62
2:B:277:VAL:CG2	2:B:294:ARG:HH11	2.12	0.62
2:B:149:ARG:NH1	2:B:149:ARG:HG3	2.14	0.62
2:B:93:GLN:NE2	2:B:96:ARG:HH11	1.90	0.62
2:B:198:THR:HA	3:B:389:HOH:O	1.99	0.61
2:B:294:ARG:NH1	2:B:316:GLN:NE2	2.44	0.61
2:B:340:PRO:HB3	3:B:479:HOH:O	2.00	0.61
2:B:65:LYS:HA	2:B:68:ARG:NH1	2.15	0.61
2:B:65:LYS:HD3	2:B:130:ILE:HD13	1.82	0.61
2:B:199:ILE:HG22	3:B:526:HOH:O	2.00	0.61
2:B:49:GLY:O	2:B:116:ARG:HD2	2.01	0.60
2:B:88:LEU:HB2	2:B:89:PRO:HD3	1.83	0.60
2:B:203:LYS:HD3	2:B:203:LYS:N	2.17	0.59
2:B:157:ILE:HG22	2:B:161:MET:HE2	1.86	0.58
2:B:158:PHE:HA	2:B:161:MET:HE3	1.85	0.58
2:B:58:LYS:HG2	3:B:513:HOH:O	2.04	0.58
2:B:144:ASN:O	2:B:149:ARG:NH2	2.37	0.58
2:B:143:GLU:O	2:B:144:ASN:HB2	2.04	0.58
1:A:53:ASN:OD1	2:B:80:SER:HB2	2.03	0.58
1:A:56:THR:O	2:B:317:THR:CG2	2.51	0.57
2:B:203:LYS:H	2:B:203:LYS:CE	2.18	0.57
2:B:349:LEU:C	2:B:351:GLY:H	2.06	0.57
2:B:320:HIS:HE1	3:B:387:HOH:O	1.87	0.57
2:B:271:PHE:HE2	3:B:497:HOH:O	1.88	0.57
2:B:164:GLU:HB3	3:B:517:HOH:O	2.04	0.56
2:B:258:TRP:N	3:B:511:HOH:O	2.37	0.56
2:B:83:TYR:HE1	3:B:566:HOH:O	1.88	0.56
2:B:158:PHE:HA	2:B:161:MET:CE	2.36	0.56
2:B:158:PHE:CD1	2:B:161:MET:HE3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ARG:NH1	2:B:101:ARG:HB3	2.17	0.54
2:B:65:LYS:HA	2:B:68:ARG:HH11	1.73	0.53
2:B:265:HIS:CE1	3:B:479:HOH:O	2.61	0.53
2:B:68:ARG:HG3	2:B:69:LEU:H	1.73	0.53
2:B:269:MET:HE2	2:B:272:LEU:CD1	2.38	0.53
1:A:59:PRO:HG3	2:B:307:TYR:OH	2.08	0.53
2:B:125:LYS:NZ	3:B:433:HOH:O	2.40	0.53
2:B:157:ILE:O	2:B:161:MET:HG3	2.08	0.53
2:B:216:SER:N	3:B:455:HOH:O	2.42	0.53
2:B:203:LYS:HE2	2:B:203:LYS:H	1.75	0.51
1:A:58:GLY:CA	2:B:317:THR:HG21	2.35	0.51
2:B:203:LYS:CD	2:B:203:LYS:N	2.73	0.51
2:B:224:LEU:HD11	2:B:228:ILE:HD11	1.91	0.51
2:B:50:THR:HA	2:B:116:ARG:HD2	1.93	0.51
2:B:287:LYS:HZ1	2:B:344:ASN:ND2	2.09	0.51
2:B:101:ARG:NH1	2:B:101:ARG:CG	2.68	0.50
2:B:340:PRO:HD3	2:B:346:ASN:ND2	2.22	0.50
2:B:269:MET:HE2	2:B:272:LEU:HD11	1.93	0.50
1:A:52:THR:N	3:A:67:HOH:O	2.45	0.50
2:B:287:LYS:NZ	2:B:344:ASN:ND2	2.61	0.49
2:B:307:TYR:HA	3:B:510:HOH:O	2.13	0.49
2:B:72:ASN:HB3	3:B:489:HOH:O	2.13	0.48
2:B:78:LYS:HZ3	2:B:78:LYS:H	1.58	0.48
2:B:203:LYS:O	2:B:207:GLN:HG3	2.13	0.48
2:B:153:LYS:O	2:B:157:ILE:HG13	2.13	0.48
2:B:68:ARG:CG	2:B:68:ARG:NH1	2.77	0.48
2:B:136:GLY:O	2:B:139:ARG:HB2	2.14	0.48
1:A:57:GLU:HG2	3:A:68:HOH:O	2.13	0.47
2:B:299:ARG:HG3	2:B:318:ILE:CD1	2.44	0.47
2:B:101:ARG:NH1	2:B:101:ARG:HG2	2.30	0.47
2:B:51:VAL:CG2	2:B:116:ARG:HA	2.45	0.47
2:B:144:ASN:CA	2:B:149:ARG:HE	2.27	0.47
2:B:185:ASP:HB3	2:B:251:TRP:CD1	2.51	0.46
2:B:78:LYS:HD3	2:B:275:ASP:OD2	2.16	0.46
2:B:77:LEU:HB3	3:B:566:HOH:O	2.16	0.46
2:B:101:ARG:HH11	2:B:101:ARG:HG2	1.78	0.45
2:B:274:TYR:HA	2:B:294:ARG:NH1	2.31	0.45
2:B:331:GLY:HA3	2:B:337:TYR:CD2	2.51	0.45
2:B:143:GLU:OE1	2:B:143:GLU:HA	2.15	0.45
2:B:345:GLN:HE21	2:B:345:GLN:CA	2.28	0.45
2:B:123:MET:HB2	2:B:123:MET:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:LEU:O	2:B:126:THR:HG23	2.16	0.45
2:B:154:LEU:HD12	2:B:157:ILE:HD12	1.99	0.45
2:B:187:ALA:O	2:B:191:ARG:HG2	2.17	0.44
2:B:277:VAL:HG21	2:B:294:ARG:NH1	2.25	0.44
2:B:153:LYS:HG3	3:B:481:HOH:O	2.17	0.44
2:B:285:ILE:HG23	2:B:286:HIS:CD2	2.53	0.44
2:B:77:LEU:CB	3:B:566:HOH:O	2.66	0.44
2:B:53:LYS:HD2	3:B:544:HOH:O	2.17	0.43
2:B:325:PHE:CE1	2:B:349:LEU:HB3	2.53	0.43
2:B:59:CYS:HB3	2:B:63:MET:CE	2.48	0.43
2:B:67:VAL:O	2:B:71:GLN:HG3	2.17	0.43
2:B:59:CYS:HB3	2:B:63:MET:HE2	2.00	0.43
2:B:149:ARG:CG	2:B:149:ARG:HH11	2.31	0.43
2:B:156:LEU:HD23	3:B:481:HOH:O	2.19	0.42
2:B:77:LEU:CD1	3:B:566:HOH:O	2.67	0.42
2:B:105:LYS:N	3:B:582:HOH:O	2.52	0.42
2:B:305:ILE:O	2:B:316:GLN:HA	2.19	0.42
2:B:225:LYS:NZ	2:B:234:ASP:HA	2.35	0.42
2:B:265:HIS:HE1	3:B:479:HOH:O	2.02	0.41
2:B:349:LEU:C	2:B:351:GLY:N	2.72	0.41
2:B:249:GLN:HB2	2:B:250:PRO:HA	2.02	0.41
2:B:52:ASP:O	2:B:56:VAL:HG23	2.20	0.41
2:B:94:HIS:HD2	3:B:543:HOH:O	2.03	0.41
2:B:85:LEU:HD22	3:B:566:HOH:O	2.19	0.41
2:B:160:HIS:HD2	3:B:497:HOH:O	2.04	0.41
2:B:234:ASP:HB3	3:B:521:HOH:O	2.20	0.41
2:B:104:GLY:C	2:B:106:MET:H	2.25	0.41
2:B:93:GLN:NE2	2:B:96:ARG:NH1	2.59	0.41
2:B:56:VAL:HG11	2:B:99:LEU:HD11	2.03	0.41
2:B:77:LEU:HA	2:B:78:LYS:NZ	2.36	0.40
2:B:62:LEU:O	2:B:66:VAL:HG23	2.20	0.40
2:B:93:GLN:NE2	2:B:96:ARG:HD3	2.36	0.40
2:B:153:LYS:HE2	3:B:467:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	6/13 (46%)	6 (100%)	0	0	100	100
2	B	302/329 (92%)	289 (96%)	11 (4%)	2 (1%)	22	16
All	All	308/342 (90%)	295 (96%)	11 (4%)	2 (1%)	25	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	270	ALA
2	B	350	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	7/11 (64%)	6 (86%)	1 (14%)	3	1
2	B	271/293 (92%)	250 (92%)	21 (8%)	13	8
All	All	278/304 (91%)	256 (92%)	22 (8%)	12	8

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
2	B	68	ARG
2	B	69	LEU
2	B	78	LYS

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Mol	Chain	Res	Type
2	B	85	LEU
2	B	96	ARG
2	B	101	ARG
2	B	103	GLU
2	B	111	GLU
2	B	134	LYS
2	B	138	GLU
2	B	142	GLU
2	B	154	LEU
2	B	173	LEU
2	B	230	LEU
2	B	272	LEU
2	B	299	ARG
2	B	317	THR
2	B	322	LYS
2	B	325	PHE
2	B	345	GLN
2	B	350	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	93	GLN
2	B	94	HIS
2	B	146	GLN
2	B	210	HIS
2	B	282	GLN
2	B	286	HIS
2	B	313	ASN
2	B	316	GLN
2	B	320	HIS
2	B	344	ASN
2	B	345	GLN
2	B	346	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	PTR	A	55	1	15,16,17	1.54	2 (13%)	19,22,24	1.07	1 (5%)

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
1	PTR	A	55	1	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	PTR	P-OH	3.15	1.64	1.59
1	A	55	PTR	CE2-CZ	2.00	1.42	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	PTR	CD2-CE2-CZ	-2.61	116.54	119.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.