



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:42 PM GMT

PDB ID : 1Q6T  
Title : THE STRUCTURE OF PHOSPHOTYROSINE PHOSPHATASE 1B IN COMPLEX WITH COMPOUND 11  
Authors : Scapin, G.; Patel, S.B.; Becker, J.W.; Wang, Q.; Despons, C.; Waddleton, D.; Skorey, K.; Cromlish, W.; Bayly, C.; Therien, M.; Gauthier, J.Y.; Li, C.S.; Lau, C.K.; Ramachandran, C.; Kennedy, B.P.; Asante-Appiah, E.  
Deposited on : 2003-08-13  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

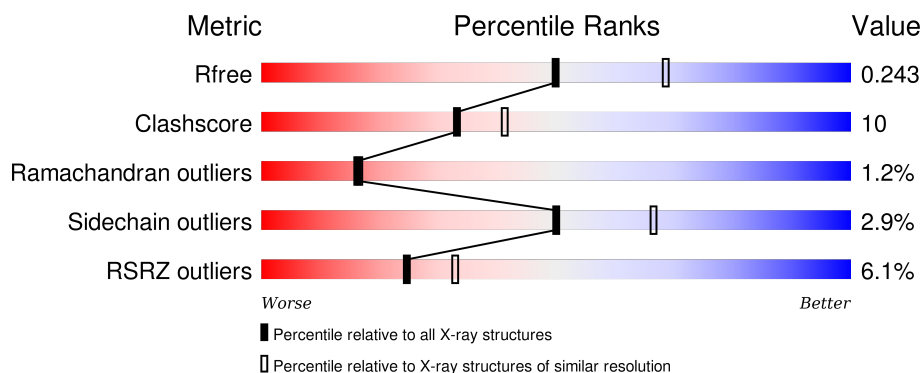
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	310	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	B	310	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5018 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-tyrosine phosphatase, non-receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2349	1490	404	439	16			
1	B	289	Total	C	N	O	S	0	0	0
			2346	1488	404	439	15			

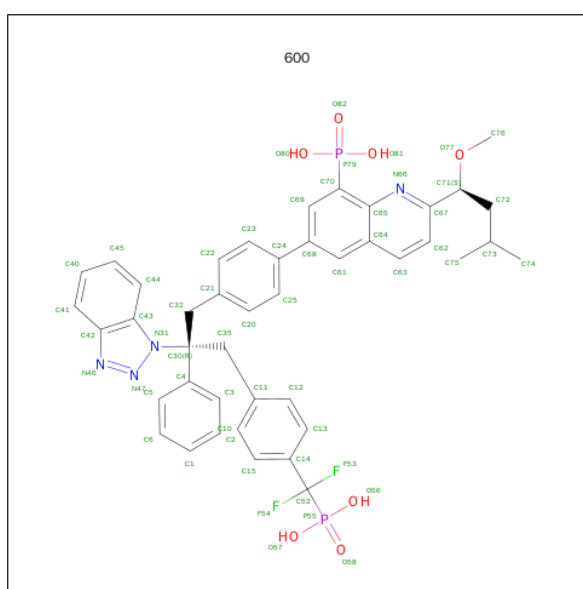
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	489	MET	-	CLONING ARTIFACT	UNP P18031
A	490	ASP	-	CLONING ARTIFACT	UNP P18031
A	491	TYR	-	CLONING ARTIFACT	UNP P18031
A	492	LYS	-	CLONING ARTIFACT	UNP P18031
A	493	ASP	-	CLONING ARTIFACT	UNP P18031
A	494	ASP	-	CLONING ARTIFACT	UNP P18031
A	495	ASP	-	CLONING ARTIFACT	UNP P18031
A	496	ASP	-	CLONING ARTIFACT	UNP P18031
A	497	LYS	-	CLONING ARTIFACT	UNP P18031
A	498	LEU	-	CLONING ARTIFACT	UNP P18031
A	499	GLU	-	CLONING ARTIFACT	UNP P18031
A	500	PHE	-	CLONING ARTIFACT	UNP P18031
B	989	MET	-	CLONING ARTIFACT	UNP P18031
B	990	ASP	-	CLONING ARTIFACT	UNP P18031
B	991	TYR	-	CLONING ARTIFACT	UNP P18031
B	992	LYS	-	CLONING ARTIFACT	UNP P18031
B	993	ASP	-	CLONING ARTIFACT	UNP P18031
B	994	ASP	-	CLONING ARTIFACT	UNP P18031
B	995	ASP	-	CLONING ARTIFACT	UNP P18031
B	996	ASP	-	CLONING ARTIFACT	UNP P18031
B	997	LYS	-	CLONING ARTIFACT	UNP P18031
B	998	LEU	-	CLONING ARTIFACT	UNP P18031
B	999	GLU	-	CLONING ARTIFACT	UNP P18031
B	1000	PHE	-	CLONING ARTIFACT	UNP P18031

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

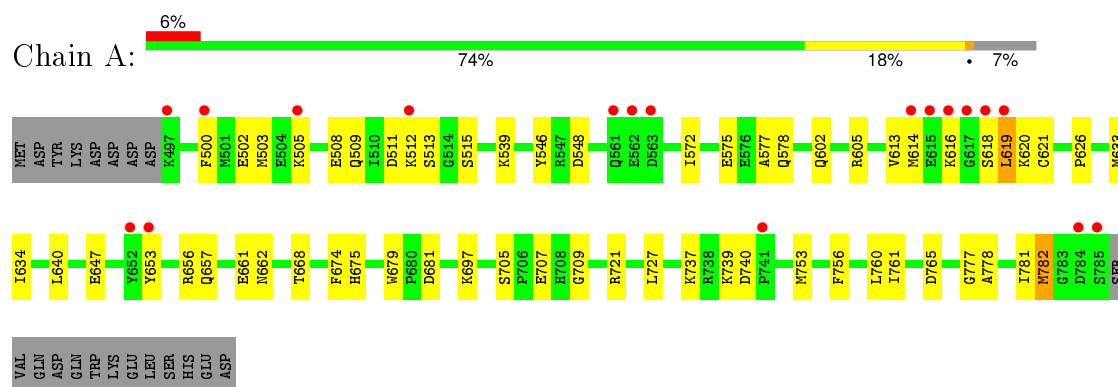
- Molecule 3 is 6-[4-((2S)-2-(1H-1,2,3-BENZOTRIAZOL-1-YL)-3-{4-[DIFLUORO(PHOSPHONO)METHYL]PHENYL}-2-PHENYLPROPYL)PHENYL]-2-[(1S)-1-METHOXY-3-METHYLBUTYL]QUINOLIN-8-YLPHOSPHONIC ACID (three-letter code: 600) (formula: C<sub>43</sub>H<sub>42</sub>F<sub>2</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>).



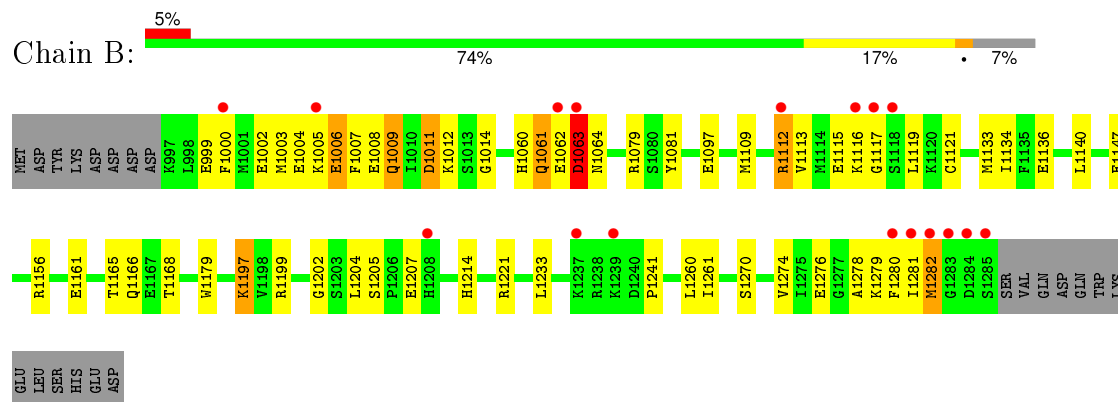
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Protein-tyrosine phosphatase, non-receptor type 1



- Molecule 1: Protein-tyrosine phosphatase, non-receptor type 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.03Å 87.83Å 138.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.30 28.38 – 1.96	Depositor EDS
% Data completeness (in resolution range)	97.4 (12.00-2.30) 90.8 (28.38-1.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 1.96Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.214 , 0.246 0.213 , 0.243	Depositor DCC
$R_{free}$ test set	2378 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.063 for k,h,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 70980 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 600

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	0.49	0/2402	0.63	0/3237
1	B	0.53	1/2399 (0.0%)	0.70	1/3234 (0.0%)
All	All	0.51	1/4801 (0.0%)	0.67	1/6471 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1119	LEU	C-N	-5.74	1.20	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1063	ASP	CA-CB-CG	-10.34	90.64	113.40

There are no chirality outliers.

There are no planarity outliers.

### 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	2349	0	2306	51	0
1	B	2346	0	2298	53	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	58	0	37	2	0
3	B	58	0	37	0	0
4	A	97	0	0	2	0
4	B	108	0	0	2	0
All	All	5018	0	4678	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (98) 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:1161:GLU:HG3	1:B:1168:THR:HG22	1.56	0.88
1:A:500:PHE:HA	1:A:503:MET:HE3	1.61	0.81
1:B:1002:GLU:HG3	1:B:1005:LYS:HE2	1.64	0.78
1:B:1112:ARG:NH1	1:B:1112:ARG:HB2	2.00	0.76
1:B:1011:ASP:O	1:B:1012:LYS:HG3	1.85	0.76
1:A:619:LEU:H	1:A:619:LEU:HD12	1.52	0.74
1:A:727:LEU:HA	1:A:753:MET:HE1	1.73	0.70
1:B:1000:PHE:HE2	1:B:1278:ALA:HB1	1.56	0.69
1:A:674:PHE:HE2	1:A:697:LYS:HD2	1.57	0.69
1:A:513:SER:HB2	1:B:1117:GLY:H	1.58	0.67
1:A:508:GLU:O	1:A:512:LYS:HG3	1.95	0.67
1:A:508:GLU:HB3	1:A:512:LYS:NZ	2.09	0.67
1:A:513:SER:HB2	1:B:1117:GLY:N	2.10	0.67
1:A:626:PRO:HG3	1:A:633:MET:HG3	1.77	0.66
1:B:1064:ASN:C	1:B:1064:ASN:OD1	2.34	0.64
1:A:605:ARG:HG2	1:A:605:ARG:HH11	1.64	0.63
1:B:1270:SER:O	1:B:1274:VAL:HG23	1.99	0.62
1:A:778:ALA:HA	1:A:781:ILE:HG22	1.82	0.62
1:A:502:GLU:HG3	1:A:505:LYS:NZ	2.16	0.61
1:B:1003:MET:O	1:B:1006:GLU:HG3	2.01	0.60
1:A:613:VAL:HG13	1:A:621:CYS:O	2.00	0.60
1:B:1002:GLU:O	1:B:1005:LYS:HG2	2.00	0.60
1:B:1113:VAL:HA	1:B:1121:CYS:HB3	1.84	0.60
1:B:1079:ARG:CZ	1:B:1233:LEU:HD11	2.33	0.59
1:A:502:GLU:HA	1:A:505:LYS:HG2	1.85	0.59
1:B:1112:ARG:HH11	1:B:1112:ARG:HB2	1.66	0.58
1:A:508:GLU:HB3	1:A:512:LYS:HZ3	1.70	0.56
1:A:619:LEU:CD1	1:A:619:LEU:H	2.16	0.56
1:B:1161:GLU:CG	1:B:1168:THR:HG22	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1205:SER:OG	1:B:1207:GLU:HG2	2.06	0.55
1:B:1063:ASP:OD1	1:B:1063:ASP:C	2.44	0.55
1:A:705:SER:OG	1:A:707:GLU:HG2	2.07	0.55
1:B:1281:ILE:HG13	1:B:1282:MET:SD	2.47	0.54
1:B:1062:GLU:OE1	1:B:1062:GLU:HA	2.06	0.54
1:B:1179:TRP:CE2	1:B:1221:ARG:HG2	2.42	0.54
1:A:619:LEU:N	1:A:619:LEU:HD12	2.20	0.54
1:A:661:GLU:HG3	1:A:668:THR:HG22	1.87	0.54
1:B:1136:GLU:HG2	4:B:190:HOH:O	2.09	0.53
1:A:778:ALA:HA	1:A:781:ILE:CG2	2.39	0.53
1:B:1112:ARG:HG2	1:B:1115:GLU:OE2	2.09	0.52
1:A:697:LYS:HD3	1:A:697:LYS:O	2.11	0.51
1:A:739:LYS:HG3	1:A:740:ASP:H	1.75	0.51
1:A:653:TYR:HB2	1:A:675:HIS:O	2.12	0.50
1:A:679:TRP:CE2	1:A:721:ARG:HG2	2.46	0.50
1:A:640:LEU:HD23	1:A:662:ASN:HA	1.93	0.50
1:A:616:LYS:NZ	1:B:1014:GLY:H	2.10	0.49
1:B:1165:THR:O	1:B:1166:GLN:HB2	2.13	0.49
1:B:1281:ILE:HG13	1:B:1282:MET:HE3	1.94	0.49
1:B:1005:LYS:HG3	1:B:1006:GLU:N	2.27	0.49
1:A:513:SER:HB2	1:B:1117:GLY:CA	2.43	0.48
1:B:1109:MET:HG3	1:B:1214:HIS:CE1	2.49	0.48
1:A:548:ASP:O	3:A:801:600:H61	2.15	0.47
1:B:1197:LYS:HE2	1:B:1197:LYS:CA	2.45	0.47
1:B:1005:LYS:CG	1:B:1006:GLU:N	2.78	0.46
1:A:502:GLU:HG3	1:A:505:LYS:HZ2	1.80	0.46
1:A:502:GLU:HG3	1:A:505:LYS:HZ3	1.81	0.46
1:A:572:ILE:HG13	1:A:756:PHE:HB2	1.97	0.46
1:B:1060:HIS:O	1:B:1061:GLN:O	2.34	0.46
1:A:614:MET:HG2	1:A:619:LEU:HG	1.98	0.45
1:B:1133:MET:C	1:B:1134:ILE:HD12	2.37	0.45
1:B:1005:LYS:HA	1:B:1008:GLU:OE2	2.17	0.45
1:B:1063:ASP:OD1	1:B:1063:ASP:O	2.33	0.45
1:A:539:LYS:HE3	4:A:36:HOH:O	2.17	0.45
1:A:515:SER:HA	4:A:29:HOH:O	2.17	0.45
1:B:1202:GLY:O	1:B:1205:SER:HB3	2.17	0.44
1:A:781:ILE:HG23	1:A:782:MET:SD	2.57	0.44
1:B:1004:GLU:O	1:B:1008:GLU:HG3	2.18	0.44
1:B:1112:ARG:CZ	1:B:1112:ARG:HB2	2.48	0.44
1:B:1276:GLU:OE1	1:B:1279:LYS:HE2	2.18	0.44
1:A:739:LYS:HG3	1:A:740:ASP:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:LYS:C	1:A:697:LYS:HD3	2.39	0.43
1:A:546:TYR:HB3	3:A:801:600:N47	2.34	0.43
1:A:513:SER:HB2	1:B:1117:GLY:HA3	2.01	0.43
1:B:999:GLU:OE2	1:B:1241:PRO:HB2	2.18	0.43
1:A:727:LEU:CA	1:A:753:MET:HE1	2.46	0.42
1:A:605:ARG:HG2	1:A:605:ARG:NH1	2.31	0.42
1:B:1005:LYS:HA	1:B:1008:GLU:CD	2.40	0.42
1:B:1278:ALA:O	1:B:1282:MET:HB2	2.19	0.42
1:B:1147:GLU:CB	1:B:1156:ARG:HG2	2.49	0.42
1:B:1147:GLU:HG3	1:B:1147:GLU:O	2.19	0.42
1:B:1079:ARG:HG2	1:B:1081:TYR:CZ	2.55	0.42
1:A:777:GLY:O	1:A:781:ILE:HG22	2.20	0.42
1:A:647:GLU:HB2	1:A:656:ARG:HG2	2.02	0.42
1:A:577:ALA:O	1:A:578:GLN:HB2	2.20	0.42
1:A:634:ILE:N	1:A:634:ILE:HD12	2.35	0.42
1:A:602:GLN:O	1:A:709:GLY:HA3	2.19	0.42
1:A:778:ALA:CA	1:A:781:ILE:HG22	2.49	0.41
1:B:1004:GLU:O	1:B:1007:PHE:HB3	2.21	0.41
1:A:618:SER:O	1:A:620:LYS:HG3	2.21	0.41
1:B:1112:ARG:HG2	1:B:1115:GLU:CD	2.41	0.41
1:B:1009:GLN:HB3	1:B:1009:GLN:HE21	1.69	0.41
1:B:1097:GLU:HA	1:B:1140:LEU:HD11	2.03	0.41
1:B:1199:ARG:HG2	1:B:1204:LEU:HD12	2.03	0.40
1:A:674:PHE:CE2	1:A:697:LYS:HD2	2.47	0.40
1:B:1064:ASN:HA	4:B:91:HOH:O	2.21	0.40
1:B:1079:ARG:NE	1:B:1233:LEU:HD11	2.36	0.40
1:A:616:LYS:HE3	1:A:681:ASP:OD1	2.22	0.40
1:A:616:LYS:HZ2	1:B:1014:GLY:H	1.70	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	287/310 (93%)	270 (94%)	14 (5%)	3 (1%)	19	21
1	B	287/310 (93%)	270 (94%)	13 (4%)	4 (1%)	14	13
All	All	574/620 (93%)	540 (94%)	27 (5%)	7 (1%)	16	16

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1061	GLN
1	B	1116	LYS
1	A	619	LEU
1	B	1011	ASP
1	A	575	GLU
1	A	761	ILE
1	B	1261	ILE

### 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	259/283 (92%)	252 (97%)	7 (3%)	52	70
1	B	258/283 (91%)	250 (97%)	8 (3%)	47	64
All	All	517/566 (91%)	502 (97%)	15 (3%)	50	66

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	509	GLN
1	A	511	ASP
1	A	657	GLN
1	A	737	LYS
1	A	760	LEU
1	A	765	ASP
1	A	782	MET
1	B	1006	GLU
1	B	1009	GLN

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Mol	Chain	Res	Type
1	B	1063	ASP
1	B	1112	ARG
1	B	1197	LYS
1	B	1260	LEU
1	B	1280	PHE
1	B	1282	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1009	GLN
1	B	1139	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 carbohydrates 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
3	600	A	801	-	55,64,64	3.60	36 (65%)	71,97,97	3.35	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	600	B	1301	-	55,64,64	3.60	32 (58%)	71,97,97	3.30	14 (19%)

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
3	600	A	801	-	-	0/42/57/57	0/7/7/7
3	600	B	1301	-	-	0/42/57/57	0/7/7/7

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	600	C67-C71	-15.27	1.42	1.51
3	B	1301	600	C67-C71	-15.13	1.42	1.51
3	B	1301	600	P55-O57	-4.35	1.46	1.54
3	B	1301	600	P79-O81	-4.32	1.45	1.54
3	A	801	600	O77-C76	-4.20	1.26	1.42
3	A	801	600	P79-O81	-4.01	1.46	1.54
3	B	1301	600	O77-C76	-3.96	1.27	1.42
3	A	801	600	P55-O57	-3.72	1.47	1.54
3	A	801	600	O77-C71	-2.48	1.29	1.42
3	B	1301	600	O77-C71	-2.37	1.30	1.42
3	A	801	600	C61-C64	2.01	1.46	1.42
3	A	801	600	C23-C24	2.02	1.43	1.39
3	B	1301	600	C2-C3	2.05	1.43	1.38
3	A	801	600	C25-C20	2.20	1.42	1.38
3	A	801	600	C69-C68	2.21	1.43	1.39
3	B	1301	600	C25-C20	2.24	1.42	1.38
3	A	801	600	C2-C1	2.27	1.43	1.38
3	A	801	600	P79-O82	2.36	1.55	1.50
3	B	1301	600	C25-C24	2.36	1.44	1.39
3	B	1301	600	C2-C1	2.39	1.44	1.38
3	A	801	600	C6-C5	2.39	1.43	1.38
3	B	1301	600	C22-C21	2.44	1.44	1.38
3	A	801	600	C45-C40	2.46	1.44	1.38
3	B	1301	600	C23-C24	2.49	1.44	1.39
3	B	1301	600	C6-C5	2.50	1.44	1.38
3	A	801	600	C22-C21	2.52	1.44	1.38
3	A	801	600	C25-C24	2.60	1.44	1.39
3	A	801	600	C32-C30	2.62	1.58	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1301	600	C12-C11	2.62	1.44	1.38
3	B	1301	600	C13-C12	2.79	1.43	1.38
3	A	801	600	C20-C21	2.83	1.44	1.38
3	A	801	600	C13-C12	2.83	1.43	1.38
3	B	1301	600	C10-C11	2.88	1.44	1.38
3	B	1301	600	C45-C40	2.97	1.45	1.38
3	B	1301	600	C13-C14	2.99	1.43	1.39
3	B	1301	600	C40-C41	2.99	1.43	1.36
3	A	801	600	C15-C14	3.00	1.44	1.39
3	B	1301	600	C67-N66	3.02	1.35	1.32
3	A	801	600	C68-C24	3.03	1.56	1.49
3	B	1301	600	C35-C11	3.08	1.56	1.51
3	A	801	600	C40-C41	3.09	1.43	1.36
3	A	801	600	C10-C11	3.11	1.45	1.38
3	B	1301	600	C63-C62	3.21	1.43	1.36
3	B	1301	600	C61-C68	3.22	1.46	1.38
3	A	801	600	C45-C44	3.23	1.44	1.36
3	A	801	600	C43-C42	3.26	1.47	1.40
3	B	1301	600	C20-C21	3.33	1.45	1.38
3	A	801	600	C61-C68	3.40	1.46	1.38
3	A	801	600	C12-C11	3.42	1.46	1.38
3	A	801	600	C63-C62	3.43	1.43	1.36
3	B	1301	600	C45-C44	3.78	1.45	1.36
3	B	1301	600	C43-C42	3.89	1.48	1.40
3	A	801	600	C62-C67	3.92	1.46	1.38
3	B	1301	600	C62-C67	4.44	1.47	1.38
3	B	1301	600	C3-C4	4.45	1.46	1.39
3	A	801	600	C13-C14	4.46	1.46	1.39
3	A	801	600	C67-N66	4.63	1.37	1.32
3	A	801	600	C64-C65	4.93	1.49	1.42
3	A	801	600	C35-C30	4.98	1.61	1.55
3	A	801	600	C32-C21	5.03	1.60	1.51
3	A	801	600	C3-C4	5.09	1.47	1.39
3	B	1301	600	C64-C65	5.22	1.49	1.42
3	A	801	600	C5-C4	5.29	1.47	1.39
3	B	1301	600	C32-C21	5.81	1.61	1.51
3	B	1301	600	C5-C4	5.91	1.48	1.39
3	B	1301	600	C35-C30	6.09	1.62	1.55
3	A	801	600	C30-C4	6.43	1.60	1.52
3	B	1301	600	C30-C4	6.75	1.60	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1301	600	C43-C42-N46	-4.07	103.29	108.55
3	A	801	600	C43-C42-N46	-3.75	103.71	108.55
3	A	801	600	C64-C65-N66	-3.37	117.91	122.64
3	A	801	600	C62-C67-N66	-3.07	119.92	123.00
3	B	1301	600	C62-C67-N66	-3.04	119.95	123.00
3	B	1301	600	C64-C65-N66	-2.93	118.53	122.64
3	B	1301	600	C69-C68-C24	-2.70	116.31	120.90
3	B	1301	600	C32-C21-C20	-2.25	117.87	121.08
3	B	1301	600	C25-C24-C68	-2.16	117.51	121.39
3	A	801	600	C70-C65-C64	2.05	120.75	118.47
3	B	1301	600	C70-C65-C64	2.05	120.76	118.47
3	B	1301	600	O81-P79-C70	2.17	110.51	106.70
3	A	801	600	C30-C35-C11	2.20	120.40	115.90
3	A	801	600	O81-P79-C70	2.21	110.57	106.70
3	A	801	600	C41-C42-N46	2.61	134.62	130.22
3	B	1301	600	C41-C42-N46	2.81	134.96	130.22
3	B	1301	600	C74-C73-C72	2.89	121.84	111.11
3	A	801	600	C76-O77-C71	2.90	122.91	113.74
3	B	1301	600	C76-O77-C71	3.05	123.38	113.74
3	A	801	600	C74-C73-C72	3.46	123.95	111.11
3	B	1301	600	C30-C32-C21	3.73	123.55	115.90
3	A	801	600	C30-C32-C21	4.24	124.60	115.90
3	A	801	600	C44-C43-N31	7.36	139.15	131.97
3	B	1301	600	C44-C43-N31	7.65	139.43	131.97
3	B	1301	600	C73-C72-C71	23.70	153.31	114.95
3	A	801	600	C73-C72-C71	24.53	154.66	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	600	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	289/310 (93%)	0.36	18 (6%) 24 32	23, 38, 68, 76	0
1	B	289/310 (93%)	0.41	17 (5%) 26 34	21, 38, 70, 78	0
All	All	578/620 (93%)	0.38	35 (6%) 25 33	21, 39, 70, 78	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1285	SER	16.2
1	A	618	SER	8.3
1	A	619	LEU	6.9
1	B	1117	GLY	5.9
1	A	785	SER	5.4
1	B	1063	ASP	5.2
1	B	1000	PHE	5.0
1	A	617	GLY	4.6
1	B	1284	ASP	4.4
1	A	652	TYR	4.2
1	B	1005	LYS	4.0
1	A	500	PHE	3.9
1	A	616	LYS	3.8
1	A	497	LYS	3.8
1	B	1062	GLU	3.8
1	A	614	MET	3.6
1	A	784	ASP	3.4
1	A	562	GLU	3.3
1	B	1237	LYS	3.3
1	A	741	PRO	3.3
1	B	1239	LYS	3.2
1	A	505	LYS	3.2
1	B	1116	LYS	3.2
1	A	563	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1282	MET	2.9
1	B	1280	PHE	2.8
1	A	561	GLN	2.7
1	B	1208	HIS	2.7
1	A	615	GLU	2.6
1	B	1118	SER	2.6
1	A	512	LYS	2.6
1	A	653	TYR	2.4
1	B	1112	ARG	2.1
1	B	1281	ILE	2.1
1	B	1283	GLY	2.1

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	600	B	1301	58/58	0.94	0.15	1.08	19,28,44,47	0
3	600	A	801	58/58	0.96	0.17	1.03	22,28,55,59	0
2	MG	B	5000	1/1	0.84	0.12	-	26,26,26,26	1
2	MG	A	6000	1/1	0.95	0.20	-	32,32,32,32	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.