

wwPDB X-ray Structure Validation Summary Report (i)

Jun 30, 2021 - 04:15 am BST

382A
3

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

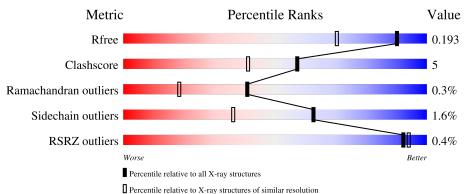
MolProbity		
9		1.8.5 (274361), CSD as541be (2020)
\mathbf{X} triage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 >=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 <=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	А	646	81%	9%	•	9%
1	В	646	80%	10%	•	9%



2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 10392 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 Nitrous-oxide reductase.

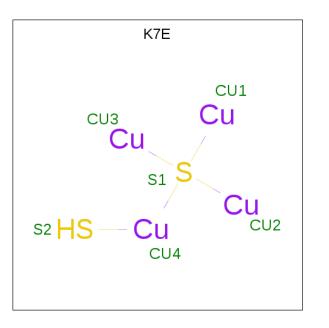
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	585	Total	С	Ν	Ο	\mathbf{S}	0	4	0
	505	4615	2919	792	872	32	0	4	0	
1	р	586	Total	С	Ν	Ο	S	0	1	0
	1 B	500	4614	2919	794	869	32	0		

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	ALA	HIS	engineered mutation	UNP P19573
А	639	TRP	-	expression tag	UNP P19573
A	640	SER	-	expression tag	UNP P19573
A	641	HIS	-	expression tag	UNP P19573
A	642	PRO	_	expression tag	UNP P19573
A	643	GLN	-	expression tag	UNP P19573
A	644	PHE	-	expression tag	UNP P19573
A	645	GLU	-	expression tag	UNP P19573
A	646	LYS	-	expression tag	UNP P19573
В	382	ALA	HIS	engineered mutation	UNP P19573
В	639	TRP	-	expression tag	UNP P19573
В	640	SER	-	expression tag	UNP P19573
В	641	HIS	-	expression tag	UNP P19573
В	642	PRO	-	expression tag	UNP P19573
В	643	GLN	-	expression tag	UNP P19573
В	644	PHE	-	expression tag	UNP P19573
В	645	GLU	-	expression tag	UNP P19573
В	646	LYS	-	expression tag	UNP P19573

There are 18 discrepancies between the modelled and reference sequences:

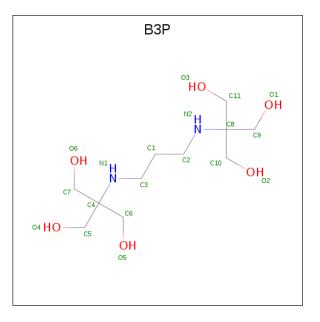
• Molecule 2 is sulfanyl-(tricuprio- $l^{4}-sulfanyl$)copper (three-letter code: K7E) (formula: Cu_4HS_2) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	At	oms		ZeroOcc	AltConf
2	А	1	Total 6	Cu 4	${ m S} { m 2}$	0	0

• Molecule 3 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: C₁₁H₂₆N₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C N O 19 11 2 6	0	0
3	В	1	Total C N O 19 11 2 6	0	0



• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Na 1 1	0	0

• Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Ca 1 1	0	0
5	В	1	Total Ca 1 1	0	0

• Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total K 1 1	0	0
6	В	1	Total K 1 1	0	0

• Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	2	Total Cl 2 2	0	0
7	В	1	Total Cl 1 1	0	0

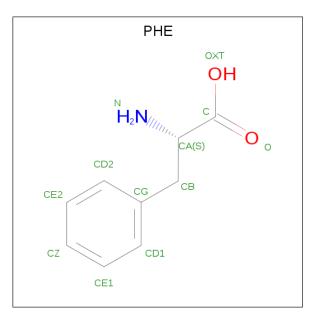
• Molecule 8 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



CUA	
cu1 <mark>Cu</mark> — <mark>Cu</mark> cu2	

ſ	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	8	А	1	Total Cu 2 2	0	0
	8	В	1	Total Cu 2 2	0	0

 $\bullet\,$ Molecule 9 is PHENYLALANINE (three-letter code: PHE) (formula: ${\rm C_9H_{11}NO_2}).$

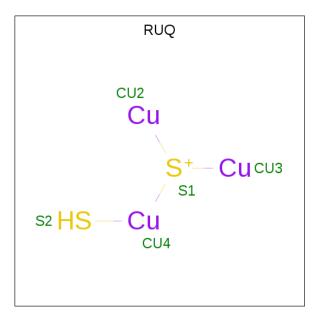


]	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	9	В	1	Total C N O 11 9 1 1	0	0

• Molecule 10 is (dicuprio- $l^{3}-sulfanyl)-sulfanyl-copper (three-letter code: RUQ) (formula:$

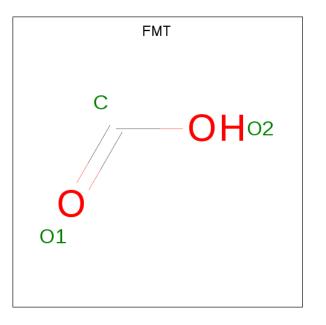


 Cu_3HS_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
10	В	1	Total 5	Cu 3	$\frac{S}{2}$	0	0

• Molecule 11 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	В	1	Total C 3 1	0 2	0	0

• Molecule 12 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	А	597	Total O 597 597	0	0
12	В	491	Total O 491 491	0	0



3 Residue-property plots (i)

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: 81%		9% • 9%
MET NET SER ASP ASP ASP SER ASP ASP CLN VAL CLN VAL CLN VAL CLN VAL CLN VAL CLN VAL CLN CLN VAL CLN CLN CLN CLN CLN ARC CLN ACC ACC ACC ACC ACC ACC ACC ACC ACC AC	VAL THR GLY ALA ALA ALA ALA ALA ALA ALA ALA GLY GLY GLY MET MET MET MET MET MET MET MET	SER TRP ALA GLN ALA K54 K54 K54 K54 K54 K54 K54 K57 K57 K57
M90 P97 V101 V101 M107 M107 M124 M126 0126 0126 0126 0127 0128 M129 M129 M129 M129 M129 M129 M126 M129 M176	H178 D204 0206 R206 R206 R269 V283 V283 V283 V283 V283 V283	K308 K311 K342 C347 C347 L355 L355
P366 73 89 8373 8373 8373 8373 8373 8373 8373 8373 8373 8373 8373 8373 8373 8373 8364 8365 8465 8465 8466 <td>N513 N543 K543 B559 B559 B559 B595 T604 T604 L613</td> <td>W620 F621 A632 A638 A638 A638 A638 A638 A638 A14 F12 F11 F11 F11</td>	N513 N543 K543 B559 B559 B559 B595 T604 T604 L613	W620 F621 A632 A638 A638 A638 A638 A638 A638 A14 F12 F11 F11 F11
LYS		
• Molecule 1: Nitrous-oxide reductase		
Chain B: 80%		10% • 9%
MET ASP ASP SER ASP SER L175 L175 C121 C121 C121 C121 C121 C121 C121 C12	VAL VAL GINY ALA ALA ALA ALA ALA ALA CLEU GIN CLEU CLEU CLEU CLEU CLEU CLEU CLEU CLEU	SER ALA ALA CILN CILN CILN CILN CILN CILN CILN CILN
	•	
H61 V87 V87 V87 V87 V101 L124 H129 H128 H128 H128 L132 L132 L132 L132 L132 L132 L132 C255 C255	V283 1300 1300 1333 1335 1335 1335 1335 133	D357 0361 0361 0361 0361 0361 0362 0373 0373 0373 0373 0373 0373 0373 037

• Molecule 1: Nitrous-oxide reductase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	68.82Å 76.83 Å 108.51 Å	Depositor
a, b, c, α , β , γ	90.00° 93.47° 90.00°	Depositor
Resolution (Å)	62.67 - 1.50	Depositor
Resolution (A)	108.31 - 1.50	EDS
% Data completeness	63.4(62.67-1.50)	Depositor
(in resolution range)	$63.6 \ (108.31 \text{-} 1.50)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.21 (at 1.50 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
D D.	0.156 , 0.194	Depositor
R, R_{free}	0.156 , 0.193	DCC
R_{free} test set	5616 reflections (4.87%)	wwPDB-VP
Wilson B-factor $(Å^2)$	21.0	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 45.4	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10392	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



 $^{^1 {\}rm Intensities}$ estimated from amplitudes.

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: K7E, NA, RUQ, CL, B3P, CUA, FMT, K, CA

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).

Mal	Chain	Bo	nd lengths	Bo	ond angles
Mol	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.47	0/4738	0.65	1/6413~(0.0%)
1	В	0.43	1/4732~(0.0%)	0.63	0/6411
All	All	0.45	1/9470~(0.0%)	0.64	1/12824~(0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
1	В	128	CYS	CB-SG	-5.45	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms Z		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	303	LEU	CA-CB-CG	-6.30	100.80	115.30

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	А	4615	0	4500	46	0
1	В	4614	0	4478	49	0
2	А	6	0	0	0	0
3	А	19	0	26	0	0

Continued on next page...



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	19	0	26	0	0
4	А	1	0	0	0	0
5	А	1	0	0	0	0
5	В	1	0	0	0	0
6	А	1	0	0	0	0
6	В	1	0	0	0	0
7	А	2	0	0	1	0
7	В	1	0	0	0	0
8	А	2	0	0	0	0
8	В	2	0	0	0	0
9	В	11	0	8	0	0
10	В	5	0	0	0	0
11	В	3	0	1	0	0
12	А	597	0	0	12	1
12	В	491	0	0	10	1
All	All	10392	0	9039	90	1

Continued from previous page...

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 5.

The worst 5 of 90 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:A:469[A]:GLU:HG3	1:A:492:GLU:HA	1.59	0.84
7:A:707:CL:CL	12:A:1245:HOH:O	2.35	0.81
1:B:469[A]:GLU:HG3	1:B:492:GLU:HA	1.64	0.79
1:A:225:GLU:OE2	12:A:801:HOH:O	2.01	0.78
1:A:206:LYS:NZ	12:A:802:HOH:O	2.18	0.76

All (1) 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)
12:A:1317:HOH:O	$12:B:1266:HOH:O[1_545]$	2.16	0.04



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	nalysed Favoured Allowed		Outliers	Percentiles	
1	А	587/646~(91%)	565~(96%)	20~(3%)	2(0%)	41	18
1	В	585/646~(91%)	563~(96%)	20~(3%)	2~(0%)	41	18
All	All	1172/1292~(91%)	1128~(96%)	40 (3%)	4 (0%)	41	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	342	LYS
1	А	342	LYS
1	А	176	ALA
1	В	176	ALA

5.3.2 Protein sidechains (i)

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	Rotameric Outliers	
1	А	503/544~(92%)	496~(99%)	7 (1%)	67 42
1	В	501/544~(92%)	492 (98%)	9 (2%)	59 30
All	All	1004/1088~(92%)	988~(98%)	16 (2%)	62 36

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	620	TRP
1	В	483	LEU

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	В	275	VAL
1	В	433	HIS
1	В	255	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	281	HIS
1	В	400	GLN
1	В	558	GLN
1	В	433	HIS
1	А	494	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	Bo	ond leng	ths	В	ond angles
	туре	Ullalli	Ites		Counts	RMSZ	# Z > 2	Counts	$\left \text{ RMSZ } \right \# Z > 2 $
8	CUA	А	708	1	$0,\!1,\!1$	0.00	-	-	



Mol	Type Chain Res		Dec	Link	Bond lengths			Bond angles		
	Type	Chain	ries		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	B3P	В	703	-	18, 18, 18	0.98	0	$21,\!23,\!23$	1.41	4 (19%)
9	PHE	В	701	-	10, 11, 12	0.71	0	$10,\!13,\!15$	0.19	0
3	B3P	А	702	-	18,18,18	0.84	1(5%)	$21,\!23,\!23$	0.92	0
8	CUA	В	708	1	$0,\!1,\!1$	0.00	-	-		
10	RUQ	В	702	1	$0,\!4,\!4$	0.00	-	-		
2	K7E	А	701	1	$0,\!5,\!5$	0.00	-	-		
11	FMT	В	706	-	$_{0,2,2}$	0.00	-	$0,\!1,\!1$	0.00	_

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	B3P	В	703	-	-	7/28/28/28	-
9	PHE	В	701	-	-	0/5/6/8	0/1/1/1
3	B3P	А	702	-	-	4/28/28/28	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\operatorname{\AA})$
3	А	702	B3P	C3-N1	2.12	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	В	703	B3P	O3-C11-C8	-2.94	105.68	111.63
3	В	703	B3P	O2-C10-C8	-2.38	106.81	111.63
3	В	703	B3P	C2-N2-C8	-2.21	112.94	116.08
3	В	703	B3P	O1-C9-C8	2.16	116.00	111.63

There are no chirality outliers.

5	of	11	torsion	outliers	are	listed	below:
0	O1	T T	00101011	Outiford	OUL O	motoca	

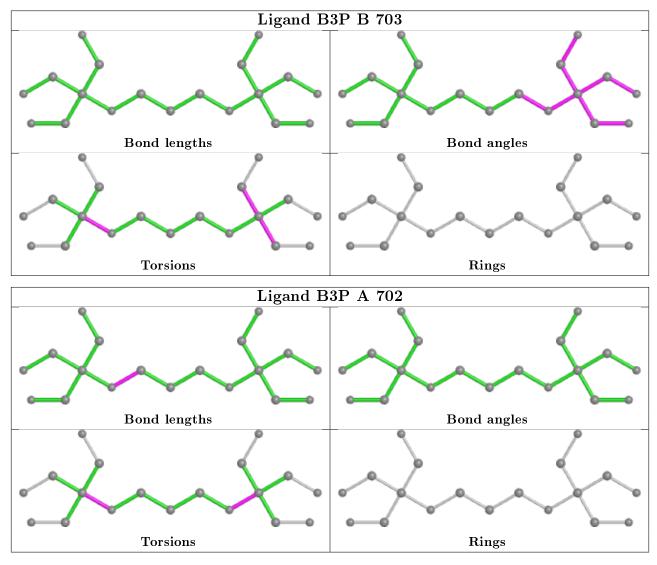
Mol	Chain	Res	Type	Atoms
3	А	702	B3P	C5-C4-N1-C3
3	А	702	B3P	C6-C4-N1-C3
3	В	703	B3P	C11-C8-C9-O1
3	В	703	B3P	O3-C11-C8-N2
3	В	703	B3P	O3-C11-C8-C9



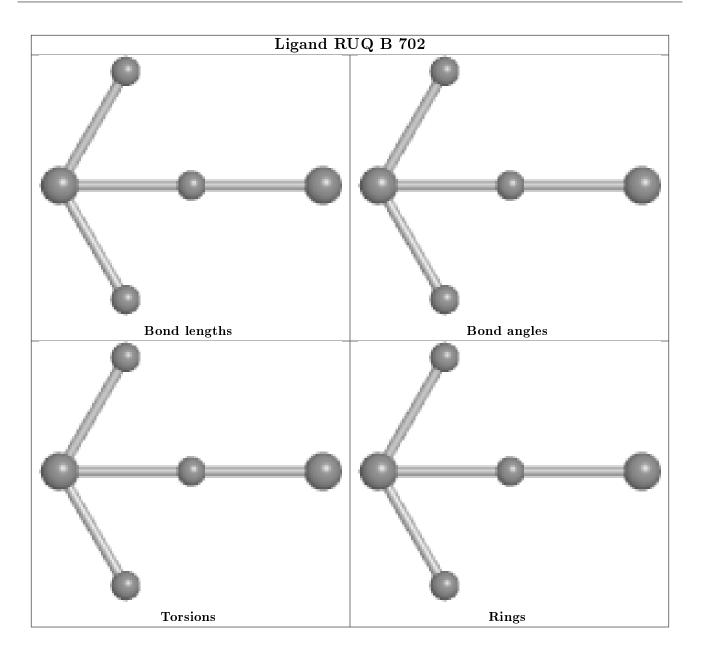
There are no ring outliers.

No monomer is involved in short contacts.

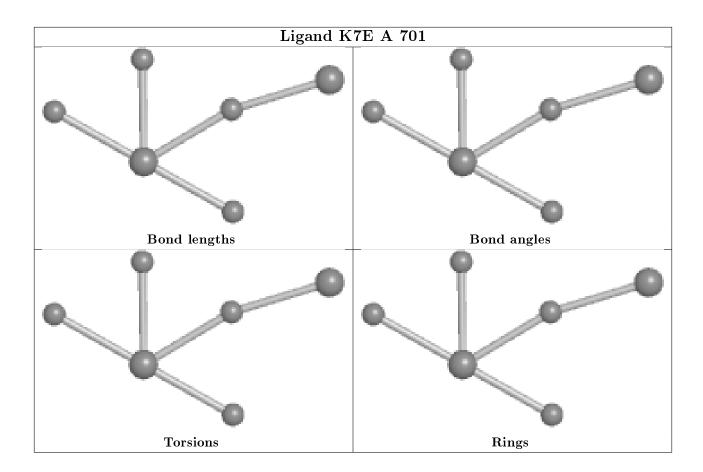
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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 $>$	$\# RSRZ {>}2$	$OWAB(A^2)$	$\mathbf{Q}{<}0.9$
1	А	585/646~(90%)	-0.60	2 (0%) 94 95	14, 23, 44, 65	0
1	В	586/646~(90%)	-0.51	3 (0%) 91 93	14, 29, 52, 74	0
All	All	1171/1292~(90%)	-0.56	5 (0%) 92 94	14, 26, 48, 74	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	360	ALA	2.5
1	А	262	PHE	2.4
1	В	309	ASP	2.3
1	В	643	GLN	2.1
1	А	269	ARG	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^{th} 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.



7	А	Q	А
		~0	

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
11	FMT	В	706	3/3	0.79	0.19	$35,\!35,\!49,\!50$	0
9	PHE	В	701	11/12	0.82	0.15	$37,\!44,\!54,\!60$	0
6	K	А	705	1/1	0.91	0.11	21,21,21,21	1
3	B3P	В	703	19/19	0.92	0.08	$22,\!28,\!34,\!48$	0
3	B3P	А	702	19/19	0.92	0.08	$24,\!28,\!32,\!35$	0
10	RUQ	В	702	5/5	0.94	0.08	$24,\!26,\!31,\!39$	5
8	CUA	В	708	2/2	0.95	0.06	32,32,32,35	1
8	CUA	А	708	2/2	0.95	0.05	$31,\!31,\!31,\!33$	0
2	K7E	А	701	6/6	0.96	0.09	$17,\!26,\!29,\!67$	6
7	CL	А	707	1/1	0.98	0.06	$31,\!31,\!31,\!31$	1
5	CA	В	704	1/1	0.98	0.08	$19,\!19,\!19,\!19$	1
5	CA	А	704	1/1	0.99	0.07	$18,\!18,\!18,\!18$	1
6	Κ	В	705	1/1	0.99	0.08	18,18,18,18	1
7	CL	А	706	1/1	0.99	0.08	24,24,24,24	1
4	NA	А	703	1/1	0.99	0.07	$19,\!19,\!19,\!19$	1
7	CL	В	707	1/1	0.99	0.07	24,24,24,24	1

6.5 Other polymers (i)

There are no such residues in this entry.

