



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2022 – 02:57 pm GMT

PDB ID : 8BB3
Title : Structure of human WDR5 and pVHL:ElonginC:ElonginB bound to PROTAC with PEG linker (conformation #1)
Authors : Kraemer, A.; Doelle, A.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2022-10-12
Resolution : 1.80 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

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>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

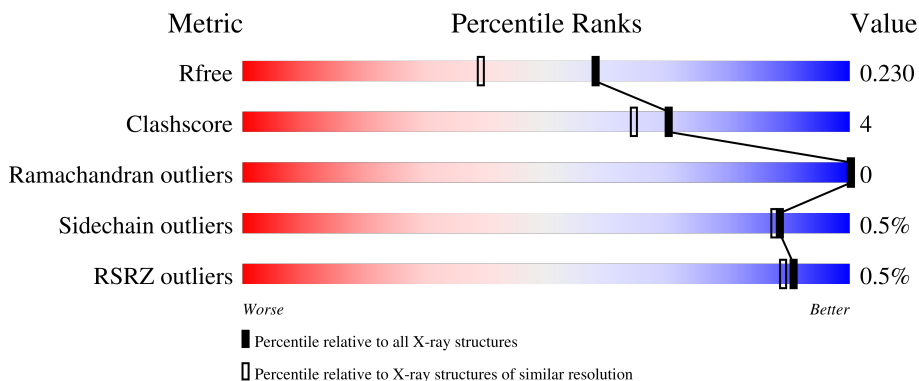
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 $\leq 5\%$. 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	J	104	99%
2	K	98	82% 7% 11%
3	L	162	90% 5% 6%
4	B	321	84% 9% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	P6G	K	201	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5513 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 Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	J	103	800	508	133	155	4	0	0	0

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	K	87	688	444	111	128	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	15	LYS	-	expression tag	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	153	1231	785	221	223	2	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	52	GLY	-	expression tag	UNP P40337
L	53	SER	-	expression tag	UNP P40337

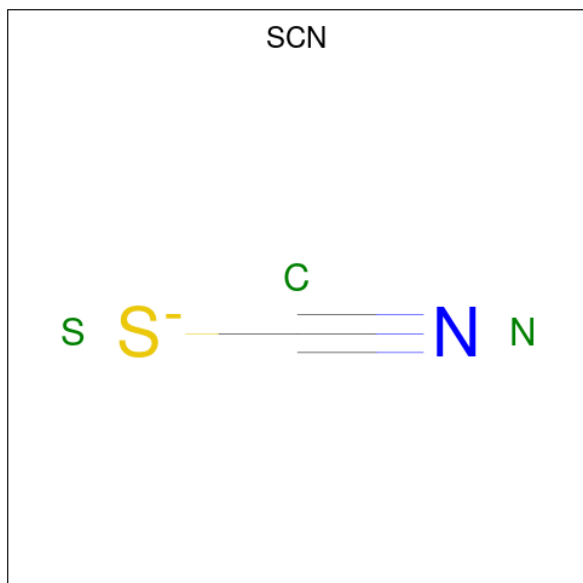
- Molecule 4 is a protein called WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	299	2290	1460	380	440	10	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	14	MET	-	initiating methionine	UNP P61964
B	15	GLY	-	expression tag	UNP P61964
B	16	SER	-	expression tag	UNP P61964
B	17	SER	-	expression tag	UNP P61964
B	18	HIS	-	expression tag	UNP P61964
B	19	HIS	-	expression tag	UNP P61964
B	20	HIS	-	expression tag	UNP P61964
B	21	HIS	-	expression tag	UNP P61964
B	22	HIS	-	expression tag	UNP P61964
B	23	HIS	-	expression tag	UNP P61964
B	24	SER	-	expression tag	UNP P61964
B	25	SER	-	expression tag	UNP P61964
B	26	GLY	-	expression tag	UNP P61964
B	27	LEU	-	expression tag	UNP P61964
B	28	VAL	-	expression tag	UNP P61964
B	29	PRO	-	expression tag	UNP P61964
B	30	ARG	-	expression tag	UNP P61964
B	31	GLY	-	expression tag	UNP P61964
B	32	SER	-	expression tag	UNP P61964

- Molecule 5 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			S
5	J	1	3	1	1	1	0	0

Continued on next page...

Continued from previous page...

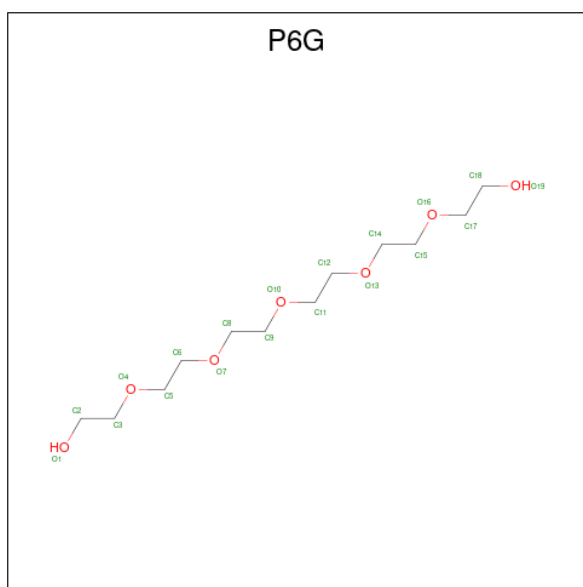
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	J	1	Total 3	C 1	N 1	S 1	0	0
5	J	1	Total 3	C 1	N 1	S 1	0	0
5	K	1	Total 3	C 1	N 1	S 1	0	0
5	L	1	Total 3	C 1	N 1	S 1	0	0
5	L	1	Total 3	C 1	N 1	S 1	0	0
5	L	1	Total 3	C 1	N 1	S 1	0	0
5	L	1	Total 3	C 1	N 1	S 1	0	0
5	L	1	Total 3	C 1	N 1	S 1	0	0
5	L	1	Total 3	C 1	N 1	S 1	0	0
5	L	1	Total 3	C 1	N 1	S 1	0	0
5	B	1	Total 3	C 1	N 1	S 1	0	0
5	B	1	Total 3	C 1	N 1	S 1	0	0
5	B	1	Total 3	C 1	N 1	S 1	0	0
5	B	1	Total 3	C 1	N 1	S 1	0	0
5	B	1	Total 3	C 1	N 1	S 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



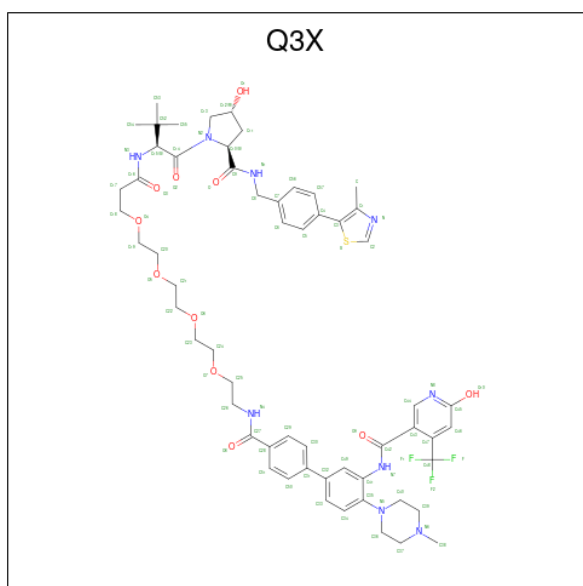
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	4	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	1	Total	C O	0	0
			19	12 7		

- Molecule 8 is {N}-[5-[4-[2-[2-[2-[2-[3-[[3,3-dimethyl-1-[(2 {S},4 {R})-2-[[4-(4-methyl-1,3-tiazol-5-yl)phenyl]methylcarbamoyl]-4-oxidanyl-pyrrolidin-1-yl]-1-oxidanylidene-butan-2-yl]amino]-3-oxidanylidene-propoxy]ethoxy]ethoxy]ethoxy]ethylcarbamoyl]phenyl]-2-(4-methylpiperazin-1-yl)phenyl]-6-oxidanylidene-4-(trifluoromethyl)-3 {H}-pyridine-3-carboxamide (three-letter code: Q3X) (formula: C₅₈H₇₂F₃N₉O₁₁S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
8	B	1	82	58	3	9	11	1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	52	Total 52	O 52	0	0
9	K	28	Total 28	O 28	0	0
9	L	86	Total 86	O 86	0	0
9	B	140	Total 140	O 140	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.

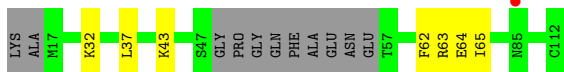
- Molecule 1: Elongin-B

Chain J:  99%



- Molecule 2: Elongin-C

Chain K:  %
82% 7% 11%




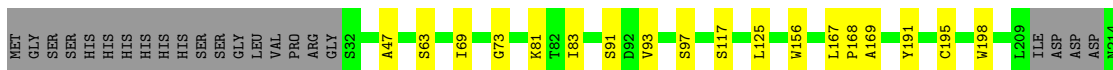
- Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain L:  90% 5% 6%



- Molecule 4: WD repeat-containing protein 5

Chain B:  %
84% 9% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.57Å 189.86Å 49.72Å 90.00° 117.64° 90.00°	Depositor
Resolution (Å)	42.91 – 1.80 42.91 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (42.91-1.80) 97.6 (42.91-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.193 , 0.227 0.196 , 0.230	Depositor DCC
R_{free} test set	3372 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtrriage
Anisotropy	0.785	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5513	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: Q3X, SCN, P6G, EDO

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	J	0.60	0/816	0.80	0/1105
2	K	0.62	0/702	0.71	0/948
3	L	0.60	0/1264	0.77	0/1727
4	B	0.64	0/2345	0.74	0/3186
All	All	0.62	0/5127	0.75	0/6966

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 [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	J	800	0	787	0	0
2	K	688	0	680	13	0
3	L	1231	0	1212	4	0
4	B	2290	0	2232	18	0
5	B	15	0	0	1	0
5	J	9	0	0	0	0
5	K	3	0	0	0	0
5	L	18	0	0	0	0
6	B	32	0	48	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	8	0	12	3	0
6	K	4	0	6	0	0
6	L	8	0	12	0	0
7	K	19	0	26	11	0
8	B	82	0	0	0	0
9	B	140	0	0	0	0
9	J	52	0	0	0	0
9	K	28	0	0	0	0
9	L	86	0	0	0	0
All	All	5513	0	5015	37	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 4.

All (37) 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:K:63:ARG:HH11	7:K:201:P6G:H31	1.51	0.75
2:K:65:ILE:HG13	7:K:201:P6G:H112	1.70	0.73
4:B:81:LYS:NZ	4:B:117:SER:O	2.26	0.68
7:K:201:P6G:H21	7:K:201:P6G:H81	1.75	0.68
6:J:204:EDO:H11	2:K:32:LYS:HE3	1.82	0.61
3:L:73:GLN:HE22	3:L:110:HIS:HD2	1.49	0.60
4:B:73:GLY:HA2	6:B:413:EDO:H22	1.86	0.57
4:B:169:ALA:HB3	4:B:198:TRP:HH2	1.71	0.56
4:B:268:VAL:HG22	6:B:414:EDO:H11	1.88	0.56
4:B:73:GLY:CA	6:B:413:EDO:H22	2.38	0.54
4:B:225:ASN:ND2	5:B:406:SCN:S	2.82	0.53
4:B:191:TYR:HA	4:B:216:PRO:HB3	1.92	0.52
3:L:176:ARG:HA	3:L:185:TYR:CE1	2.44	0.52
2:K:37:LEU:HD22	2:K:43:LYS:HG3	1.91	0.52
2:K:64:GLU:HB2	7:K:201:P6G:H111	1.91	0.51
3:L:154:PRO:HG2	3:L:156:TYR:CE1	2.46	0.51
7:K:201:P6G:O1	7:K:201:P6G:H122	2.12	0.50
2:K:63:ARG:NH1	7:K:201:P6G:H31	2.24	0.49
6:J:204:EDO:H11	2:K:32:LYS:CE	2.42	0.48
4:B:220:VAL:HA	4:B:230:LEU:O	2.15	0.47
2:K:65:ILE:HG13	7:K:201:P6G:C11	2.41	0.46
2:K:63:ARG:HD3	7:K:201:P6G:C3	2.48	0.44
4:B:215:PRO:HG2	4:B:233:THR:HB	1.99	0.44
4:B:47:ALA:HB2	4:B:322:GLU:HG3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:169:ALA:HB3	4:B:198:TRP:CH2	2.50	0.44
3:L:109:ILE:C	3:L:109:ILE:HD12	2.39	0.43
4:B:125:LEU:HB3	4:B:156:TRP:CE3	2.54	0.43
2:K:62:PHE:HD1	7:K:201:P6G:H91	1.83	0.42
6:J:204:EDO:H11	2:K:32:LYS:NZ	2.33	0.42
4:B:69:ILE:HB	4:B:83:ILE:HB	2.01	0.42
2:K:63:ARG:HD3	7:K:201:P6G:O4	2.19	0.42
2:K:63:ARG:HB2	7:K:201:P6G:C2	2.50	0.41
4:B:167:LEU:HA	4:B:168:PRO:HD3	1.83	0.41
4:B:218:SER:HB2	4:B:261:CYS:HA	2.01	0.41
4:B:195:CYS:SG	4:B:217:VAL:HG11	2.60	0.41
4:B:63:SER:HB3	4:B:93:VAL:HG13	2.02	0.41
4:B:97:SER:OG	6:B:410:EDO:H11	2.21	0.41

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	J	101/104 (97%)	95 (94%)	6 (6%)	0	100	100
2	K	83/98 (85%)	83 (100%)	0	0	100	100
3	L	152/162 (94%)	149 (98%)	3 (2%)	0	100	100
4	B	295/321 (92%)	281 (95%)	14 (5%)	0	100	100
All	All	631/685 (92%)	608 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	Outliers	Percentiles	
1	J	87/92 (95%)	87 (100%)	0	100	100
2	K	76/86 (88%)	76 (100%)	0	100	100
3	L	137/148 (93%)	136 (99%)	1 (1%)	84	81
4	B	254/280 (91%)	252 (99%)	2 (1%)	81	78
All	All	554/606 (91%)	551 (100%)	3 (0%)	88	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	69	ARG
4	B	91	SER
4	B	305	ILE

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

Mol	Chain	Res	Type
3	L	110	HIS
3	L	145	GLN

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

30 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
6	EDO	B	408	-	3,3,3	0.42	0	2,2,2	0.42	0
5	SCN	J	201	-	1,2,2	0.97	0	0,1,1	-	-
6	EDO	B	410	-	3,3,3	0.39	0	2,2,2	1.03	0
6	EDO	J	205	-	3,3,3	0.50	0	2,2,2	0.59	0
5	SCN	J	202	-	1,2,2	1.18	0	0,1,1	-	-
5	SCN	L	306	-	1,2,2	0.99	0	0,1,1	-	-
6	EDO	B	414	-	3,3,3	0.59	0	2,2,2	0.17	0
5	SCN	L	304	-	1,2,2	1.04	0	0,1,1	-	-
5	SCN	B	405	-	1,2,2	0.88	0	0,1,1	-	-
5	SCN	L	303	-	1,2,2	0.78	0	0,1,1	-	-
7	P6G	K	201	-	18,18,18	0.34	0	17,17,17	0.89	0
5	SCN	B	402	-	1,2,2	0.79	0	0,1,1	-	-
5	SCN	B	406	-	1,2,2	0.63	0	0,1,1	-	-
6	EDO	L	307	-	3,3,3	0.71	0	2,2,2	0.28	0
6	EDO	J	204	-	3,3,3	0.33	0	2,2,2	0.26	0
5	SCN	J	203	-	1,2,2	0.97	0	0,1,1	-	-
8	Q3X	B	407	-	83,88,88	0.31	0	107,123,123	0.56	0
6	EDO	B	401	-	3,3,3	0.45	0	2,2,2	0.33	0
5	SCN	K	202	-	1,2,2	1.04	0	0,1,1	-	-
6	EDO	B	409	-	3,3,3	0.47	0	2,2,2	0.75	0
5	SCN	B	403	-	1,2,2	0.67	0	0,1,1	-	-
5	SCN	B	404	-	1,2,2	0.50	0	0,1,1	-	-
6	EDO	L	308	-	3,3,3	0.50	0	2,2,2	0.55	0
6	EDO	B	411	-	3,3,3	0.47	0	2,2,2	0.56	0
6	EDO	B	413	-	3,3,3	0.44	0	2,2,2	0.37	0
5	SCN	L	302	-	1,2,2	0.18	0	0,1,1	-	-
5	SCN	L	305	-	1,2,2	0.60	0	0,1,1	-	-
6	EDO	B	412	-	3,3,3	0.44	0	2,2,2	0.38	0
5	SCN	L	301	-	1,2,2	1.20	0	0,1,1	-	-
6	EDO	K	203	-	3,3,3	0.41	0	2,2,2	0.51	0

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
6	EDO	B	408	-	-	0/1/1/1	-
6	EDO	L	308	-	-	0/1/1/1	-
6	EDO	B	411	-	-	0/1/1/1	-
6	EDO	B	413	-	-	0/1/1/1	-
6	EDO	B	410	-	-	0/1/1/1	-
7	P6G	K	201	-	-	10/16/16/16	-
8	Q3X	B	407	-	-	7/75/97/97	0/7/7/7
6	EDO	B	401	-	-	1/1/1/1	-
6	EDO	J	205	-	-	1/1/1/1	-
6	EDO	L	307	-	-	0/1/1/1	-
6	EDO	B	409	-	-	0/1/1/1	-
6	EDO	B	412	-	-	1/1/1/1	-
6	EDO	B	414	-	-	0/1/1/1	-
6	EDO	J	204	-	-	1/1/1/1	-
6	EDO	K	203	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	407	Q3X	O7-C25-C26-N4
7	K	201	P6G	O10-C11-C12-O13
8	B	407	Q3X	C25-C26-N4-C27
7	K	201	P6G	C12-C11-O10-C9
7	K	201	P6G	O1-C2-C3-O4
6	B	401	EDO	O1-C1-C2-O2
7	K	201	P6G	C5-C6-O7-C8
7	K	201	P6G	O16-C17-C18-O19
7	K	201	P6G	O4-C5-C6-O7
7	K	201	P6G	O13-C14-C15-O16
7	K	201	P6G	C14-C15-O16-C17
8	B	407	Q3X	C21-C22-O6-C23
7	K	201	P6G	C9-C8-O7-C6
8	B	407	Q3X	C26-C25-O7-C24
8	B	407	Q3X	C19-C20-O5-C21
8	B	407	Q3X	O5-C21-C22-O6

Continued on next page...

Continued from previous page...

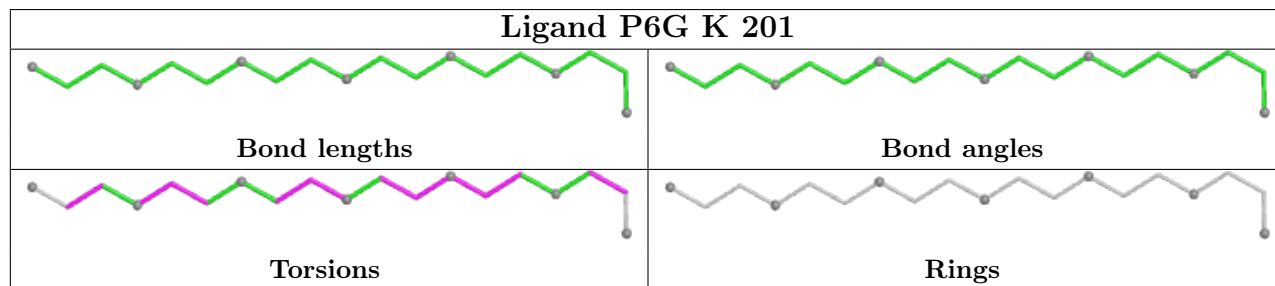
Mol	Chain	Res	Type	Atoms
6	J	205	EDO	O1-C1-C2-O2
7	K	201	P6G	O7-C8-C9-O10
6	J	204	EDO	O1-C1-C2-O2
8	B	407	Q3X	C24-C23-O6-C22
6	B	412	EDO	O1-C1-C2-O2

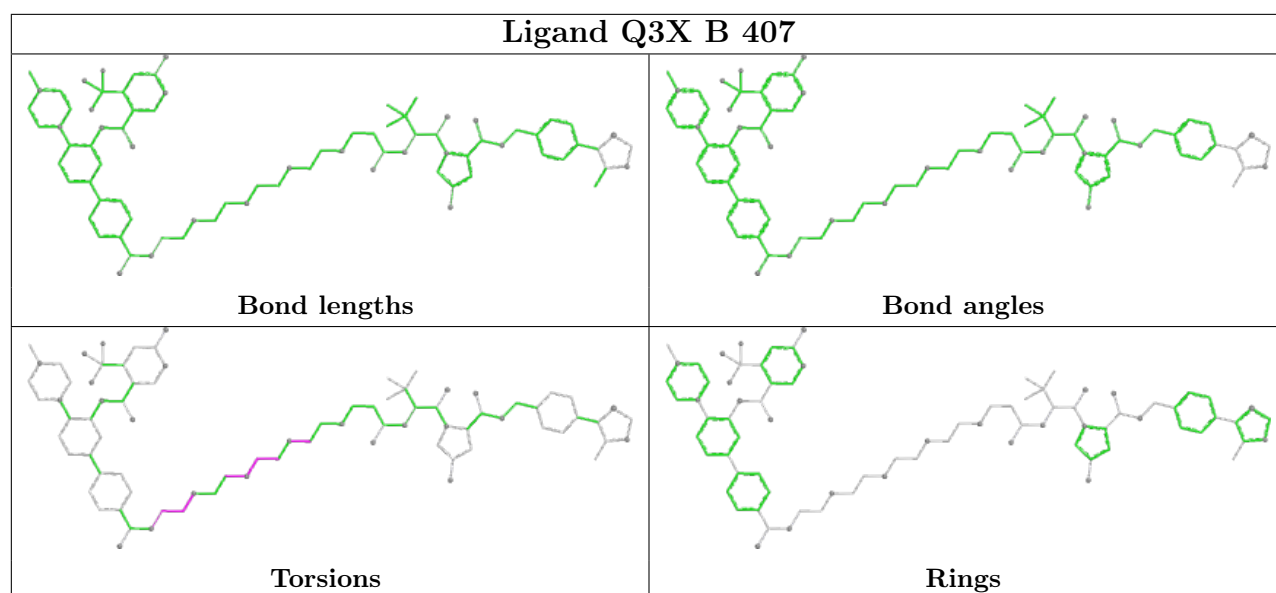
There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	410	EDO	1	0
6	B	414	EDO	1	0
7	K	201	P6G	11	0
5	B	406	SCN	1	0
6	J	204	EDO	3	0
6	B	413	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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(Å ²)	Q<0.9
1	J	103/104 (99%)	-0.28	0 100 100	23, 33, 43, 53	2 (1%)
2	K	87/98 (88%)	-0.35	1 (1%) 80 78	21, 29, 46, 53	0
3	L	153/162 (94%)	-0.30	0 100 100	22, 30, 46, 73	0
4	B	299/321 (93%)	-0.22	2 (0%) 87 86	21, 30, 43, 51	0
All	All	642/685 (93%)	-0.27	3 (0%) 91 89	21, 30, 45, 73	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	334	CYS	3.4
4	B	333	ASP	2.3
2	K	85	ASN	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 monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.