



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:00 am BST

PDB ID : 6KM7  
Title : The structural basis for the internal interaction in RBBP5  
Authors : Han, J.; Li, T.; Chen, Y.  
Deposited on : 2019-07-31  
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](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 : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

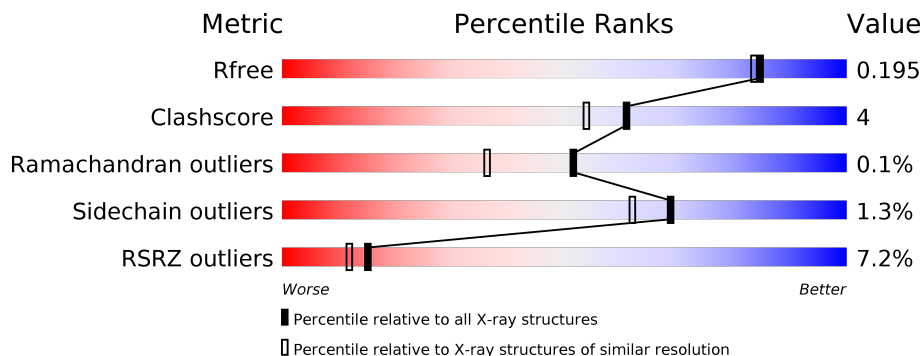
# 1 Overall quality at a glance

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 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  $\leq 5\%$ . 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	317	
1	B	317	
2	C	69	
2	D	69	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5963 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 Retinoblastoma-binding protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	313	2439	1540	431	453	15	0	0	0
1	B	312	2431	1536	429	451	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	SER	-	expression tag	UNP Q15291
B	9	SER	-	expression tag	UNP Q15291

- Molecule 2 is a protein called Retinoblastoma-binding protein 5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	32	251	164	41	46	0	1	0
2	D	34	266	175	45	46	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	deletion	UNP Q15291
C	?	-	ALA	deletion	UNP Q15291
C	?	-	VAL	deletion	UNP Q15291
C	?	-	GLN	deletion	UNP Q15291
C	?	-	THR	deletion	UNP Q15291
C	?	-	SER	deletion	UNP Q15291
C	?	-	LEU	deletion	UNP Q15291
C	?	-	MET	deletion	UNP Q15291
C	?	-	ASP	deletion	UNP Q15291
C	?	-	GLU	deletion	UNP Q15291

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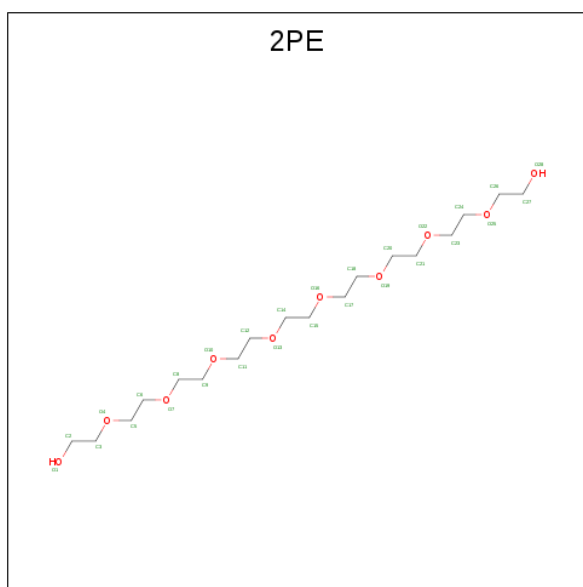
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP Q15291
C	?	-	ALA	deletion	UNP Q15291
C	?	-	SER	deletion	UNP Q15291
C	?	-	SER	deletion	UNP Q15291
C	?	-	GLU	deletion	UNP Q15291
C	?	-	LYS	deletion	UNP Q15291
C	?	-	LYS	deletion	UNP Q15291
C	?	-	ARG	deletion	UNP Q15291
C	?	-	GLN	deletion	UNP Q15291
C	?	-	SER	deletion	UNP Q15291
C	?	-	SER	deletion	UNP Q15291
C	?	-	ALA	deletion	UNP Q15291
D	?	-	ASP	deletion	UNP Q15291
D	?	-	ALA	deletion	UNP Q15291
D	?	-	VAL	deletion	UNP Q15291
D	?	-	GLN	deletion	UNP Q15291
D	?	-	THR	deletion	UNP Q15291
D	?	-	SER	deletion	UNP Q15291
D	?	-	LEU	deletion	UNP Q15291
D	?	-	MET	deletion	UNP Q15291
D	?	-	ASP	deletion	UNP Q15291
D	?	-	GLU	deletion	UNP Q15291
D	?	-	GLY	deletion	UNP Q15291
D	?	-	ALA	deletion	UNP Q15291
D	?	-	SER	deletion	UNP Q15291
D	?	-	SER	deletion	UNP Q15291
D	?	-	GLU	deletion	UNP Q15291
D	?	-	LYS	deletion	UNP Q15291
D	?	-	LYS	deletion	UNP Q15291
D	?	-	ARG	deletion	UNP Q15291
D	?	-	GLN	deletion	UNP Q15291
D	?	-	SER	deletion	UNP Q15291
D	?	-	SER	deletion	UNP Q15291
D	?	-	ALA	deletion	UNP Q15291

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



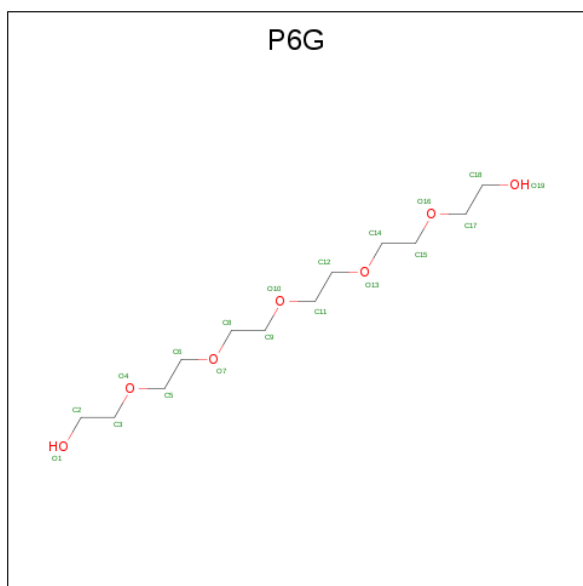
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>10</sub>).



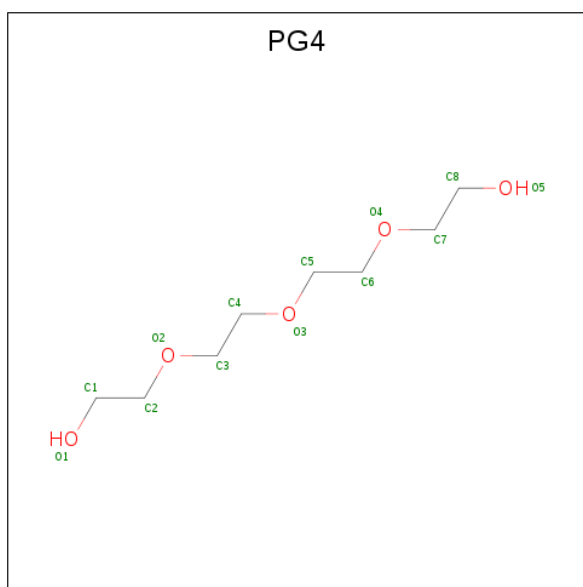
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total	C	O	0	0
			25	16	9		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			13	8	5		

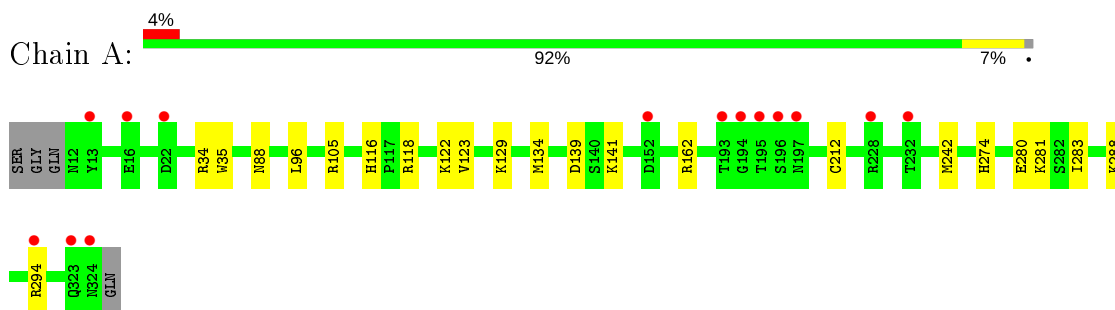
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	219	Total	O	0	0
			219	219		
7	B	212	Total	O	0	0
			212	212		
7	C	29	Total	O	0	0
			29	29		
7	D	19	Total	O	0	0
			19	19		

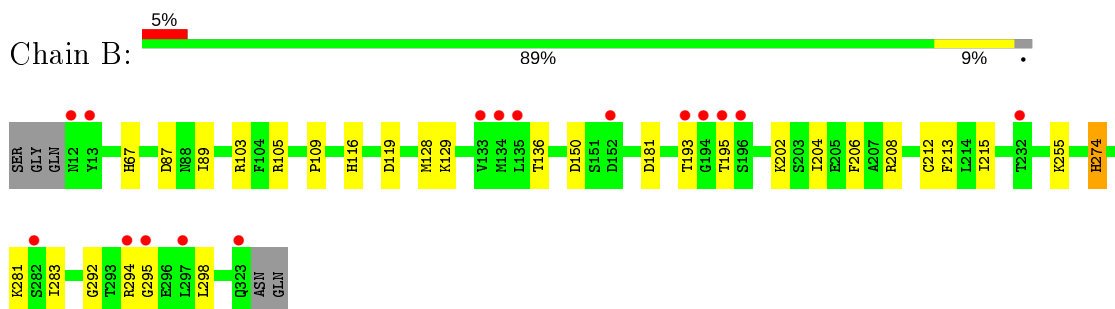
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

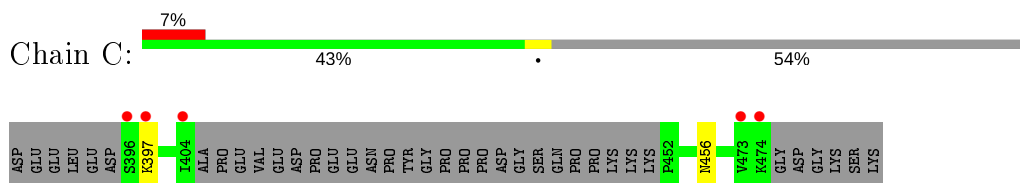
- Molecule 1: Retinoblastoma-binding protein 5



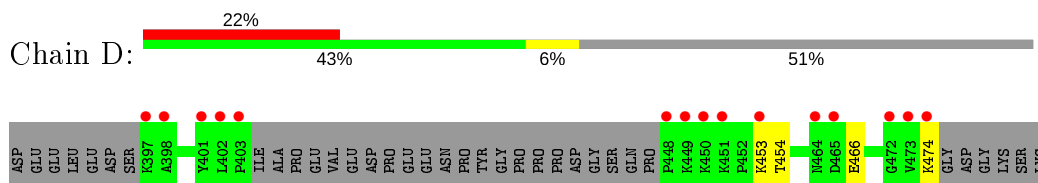
- Molecule 1: Retinoblastoma-binding protein 5



- Molecule 2: Retinoblastoma-binding protein 5



- Molecule 2: Retinoblastoma-binding protein 5





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.57Å 68.84Å 72.79Å 99.24° 99.31° 113.81°	Depositor
Resolution (Å)	34.77 – 1.80 34.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (34.77-1.80) 96.2 (34.77-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 1.81Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.165 , 0.194 0.166 , 0.195	Depositor DCC
$R_{free}$ test set	4355 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 63.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, 2PE, SO4, P6G

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	0.42	0/2491	0.61	0/3384
1	B	0.55	0/2483	0.64	0/3373
2	C	0.30	0/258	0.60	0/350
2	D	0.30	0/271	0.52	0/365
All	All	0.48	0/5503	0.62	0/7472

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	A	2439	0	2439	23	0
1	B	2431	0	2433	20	0
2	C	251	0	269	2	0
2	D	266	0	293	4	0
3	A	10	0	0	0	0
3	B	30	0	0	0	0
4	A	25	0	33	6	0
5	B	19	0	26	3	0
6	C	13	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	219	0	0	2	0
7	B	212	0	0	8	0
7	C	29	0	0	0	0
7	D	19	0	0	0	0
All	All	5963	0	5511	49	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 (49) 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:122:LYS:HB3	1:A:134:MET:HE2	1.27	1.09
1:A:116:HIS:HD2	1:A:118:ARG:H	1.27	0.83
1:A:122:LYS:HB3	1:A:134:MET:CE	2.11	0.78
1:A:212:CYS:SG	1:A:281:LYS:NZ	2.56	0.75
1:A:242:MET:CE	1:A:281:LYS:HZ3	2.02	0.72
1:A:242:MET:HE3	1:A:281:LYS:HZ3	1.56	0.71
1:B:103:ARG:NH1	2:D:454:THR:OG1	2.29	0.65
1:A:35:TRP:HA	4:A:403:2PE:H121	1.78	0.64
1:A:116:HIS:CD2	1:A:118:ARG:H	2.14	0.63
1:B:294:ARG:HD3	1:B:295:GLY:N	2.15	0.61
1:B:109:PRO:HD2	1:B:128:MET:HE3	1.83	0.60
1:A:35:TRP:CD1	4:A:403:2PE:H122	2.37	0.60
1:A:129:LYS:NZ	7:A:506:HOH:O	2.37	0.57
1:A:35:TRP:HD1	4:A:403:2PE:H122	1.68	0.57
1:A:118:ARG:HH12	1:A:162:ARG:HH11	1.51	0.57
1:B:204:ILE:HG12	1:B:215:ILE:HD12	1.87	0.57
1:B:128:MET:HE1	2:D:466:GLU:HB3	1.86	0.56
1:A:118:ARG:HH12	1:A:162:ARG:NH1	2.03	0.56
1:A:294:ARG:NH1	7:A:507:HOH:O	2.39	0.56
5:B:407:P6G:H172	7:B:569:HOH:O	2.06	0.55
1:B:193:THR:OG1	1:B:195:THR:OG1	2.24	0.54
1:B:208:ARG:NH1	7:B:501:HOH:O	2.23	0.54
1:B:202:LYS:NZ	7:B:504:HOH:O	2.41	0.53
1:A:123:VAL:N	1:A:134:MET:HE3	2.27	0.49
1:B:128:MET:CE	2:D:466:GLU:HB3	2.43	0.49
2:D:474:LYS:O	2:D:474:LYS:HG3	2.13	0.48
1:A:122:LYS:CB	1:A:134:MET:HE2	2.20	0.48
1:A:35:TRP:NE1	4:A:403:2PE:H82	2.29	0.47
5:B:407:P6G:H171	7:B:665:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLU:OE2	1:A:283:ILE:HD12	2.15	0.47
1:B:129:LYS:NZ	7:B:509:HOH:O	2.48	0.46
1:B:136:THR:HG23	7:B:614:HOH:O	2.16	0.46
1:A:139:ASP:CG	1:A:141:LYS:HD3	2.37	0.46
1:B:116:HIS:HB3	1:B:119:ASP:O	2.18	0.44
1:A:105:ARG:NE	2:C:456[A]:ASN:OD1	2.47	0.44
1:A:34:ARG:NH2	4:A:403:2PE:H81	2.32	0.43
1:B:206:PHE:CD2	1:B:213:PHE:HB3	2.54	0.43
2:C:397:LYS:HA	2:C:397:LYS:HD2	1.53	0.43
5:B:407:P6G:H141	5:B:407:P6G:H111	1.60	0.42
7:B:576:HOH:O	6:C:501:PG4:H32	2.19	0.42
1:B:274:HIS:CD2	1:B:292:GLY:HA3	2.54	0.41
1:B:89:ILE:HD11	1:B:105:ARG:CZ	2.50	0.41
1:B:67:HIS:CG	1:B:87:ASP:HB2	2.55	0.41
1:B:181:ASP:HB2	7:B:683:HOH:O	2.21	0.41
1:B:283:ILE:CG1	1:B:283:ILE:O	2.68	0.41
1:A:123:VAL:N	1:A:134:MET:CE	2.84	0.41
1:B:204:ILE:HG12	1:B:215:ILE:CD1	2.50	0.41
1:B:212:CYS:SG	1:B:281:LYS:NZ	2.64	0.40
1:A:35:TRP:HB3	4:A:403:2PE:H142	2.03	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	311/317 (98%)	304 (98%)	6 (2%)	1 (0%)	41 27
1	B	310/317 (98%)	301 (97%)	9 (3%)	0	100 100
2	C	29/69 (42%)	28 (97%)	1 (3%)	0	100 100
2	D	30/69 (44%)	30 (100%)	0	0	100 100
All	All	680/772 (88%)	663 (98%)	16 (2%)	1 (0%)	51 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ASN

### 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	A	272/275 (99%)	269 (99%)	3 (1%)	73	68
1	B	271/275 (98%)	267 (98%)	4 (2%)	65	56
2	C	30/61 (49%)	30 (100%)	0	100	100
2	D	31/61 (51%)	30 (97%)	1 (3%)	39	25
All	All	604/672 (90%)	596 (99%)	8 (1%)	69	62

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	274	HIS
1	A	288	LYS
1	B	150	ASP
1	B	255	LYS
1	B	274	HIS
1	B	298	LEU
2	D	453	LYS

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

Mol	Chain	Res	Type
1	A	116	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 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	PG4	C	501	-	12,12,12	0.54	0	11,11,11	0.33	0
3	SO4	B	404	-	4,4,4	0.12	0	6,6,6	0.13	0
4	2PE	A	403	-	24,24,27	0.53	0	23,23,26	0.31	0
3	SO4	A	402	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	B	405	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	A	401	-	4,4,4	0.15	0	6,6,6	0.10	0
3	SO4	B	401	-	4,4,4	0.14	0	6,6,6	0.30	0
3	SO4	B	406	-	4,4,4	0.14	0	6,6,6	0.07	0
5	P6G	B	407	-	18,18,18	0.53	0	17,17,17	0.51	0
3	SO4	B	402	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	B	403	-	4,4,4	0.10	0	6,6,6	0.18	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
4	2PE	A	403	-	-	13/22/22/25	-
5	P6G	B	407	-	-	9/16/16/16	-
6	PG4	C	501	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

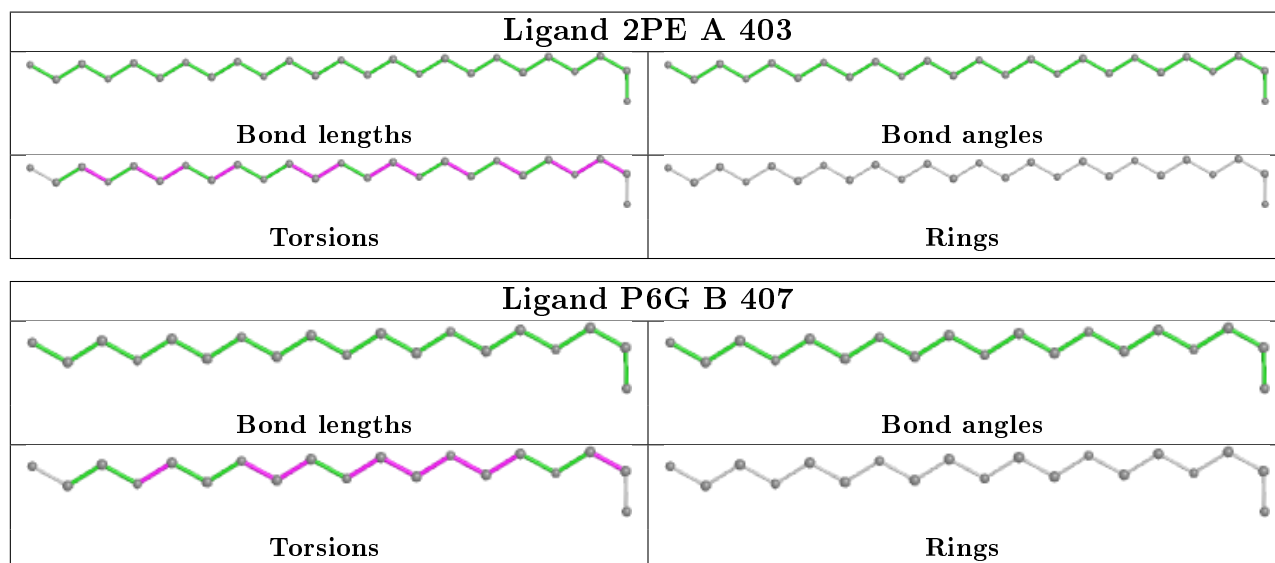
Mol	Chain	Res	Type	Atoms
5	B	407	P6G	C11-C12-O13-C14
4	A	403	2PE	O10-C11-C12-O13
6	C	501	PG4	O2-C3-C4-O3
5	B	407	P6G	C14-C15-O16-C17
6	C	501	PG4	O4-C7-C8-O5
5	B	407	P6G	O1-C2-C3-O4
5	B	407	P6G	O7-C8-C9-O10
6	C	501	PG4	O3-C5-C6-O4
6	C	501	PG4	O1-C1-C2-O2
4	A	403	2PE	O1-C2-C3-O4
4	A	403	2PE	O19-C20-C21-O22
5	B	407	P6G	O10-C11-C12-O13
4	A	403	2PE	O13-C14-C15-O16
4	A	403	2PE	C24-C23-O22-C21
4	A	403	2PE	C6-C5-O4-C3
5	B	407	P6G	C5-C6-O7-C8
4	A	403	2PE	C5-C6-O7-C8
6	C	501	PG4	C3-C4-O3-C5
4	A	403	2PE	O16-C17-C18-O19
4	A	403	2PE	O7-C8-C9-O10
4	A	403	2PE	C15-C14-O13-C12
6	C	501	PG4	C8-C7-O4-C6
4	A	403	2PE	C12-C11-O10-C9
5	B	407	P6G	C9-C8-O7-C6
5	B	407	P6G	C8-C9-O10-C11
4	A	403	2PE	C2-C3-O4-C5
4	A	403	2PE	C21-C20-O19-C18
5	B	407	P6G	O4-C5-C6-O7

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	501	PG4	1	0
4	A	403	2PE	6	0
5	B	407	P6G	3	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, 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	313/317 (98%)	-0.14	14 (4%) 33 27	14, 24, 53, 90	0
1	B	312/317 (98%)	-0.05	16 (5%) 28 22	14, 26, 55, 95	0
2	C	32/69 (46%)	0.76	5 (15%) 2 1	23, 35, 61, 96	0
2	D	34/69 (49%)	1.91	15 (44%) 0 0	28, 53, 96, 101	0
All	All	691/772 (89%)	0.05	50 (7%) 15 12	14, 26, 60, 101	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	473	VAL	9.8
1	B	195	THR	7.6
2	C	396	SER	6.8
1	A	195	THR	6.7
2	D	397	LYS	5.9
1	A	196	SER	5.7
1	B	194	GLY	5.4
2	D	474	LYS	5.1
2	D	448	PRO	4.9
2	D	472	GLY	4.8
1	A	324	ASN	4.3
1	A	194	GLY	4.3
1	B	196	SER	4.3
2	D	464	ASN	4.1
2	C	397	LYS	3.7
2	D	449	LYS	3.6
1	B	193	THR	3.5
2	C	474	LYS	3.5
1	B	232	THR	3.5
1	B	294	ARG	3.4
1	B	282	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	450	LYS	3.4
1	A	197	ASN	3.3
2	D	398	ALA	3.2
1	B	295	GLY	3.2
2	C	404	ILE	3.2
2	D	401	TYR	3.2
1	A	22	ASP	3.0
1	B	323	GLN	3.0
1	B	12	ASN	2.9
1	A	193	THR	2.9
1	A	294	ARG	2.8
2	D	465	ASP	2.6
1	B	13	TYR	2.6
1	B	134	MET	2.6
1	B	133	VAL	2.6
1	A	323	GLN	2.5
1	B	152	ASP	2.5
1	A	13	TYR	2.5
2	D	403	PRO	2.5
1	A	152	ASP	2.5
2	D	453	LYS	2.5
1	B	297	LEU	2.3
2	C	473	VAL	2.3
2	D	402	LEU	2.2
1	A	228	ARG	2.2
1	A	232	THR	2.1
1	B	135	LEU	2.1
2	D	451	LYS	2.1
1	A	16	GLU	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

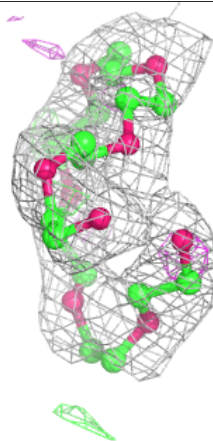
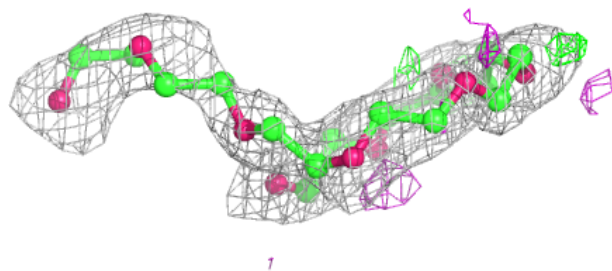
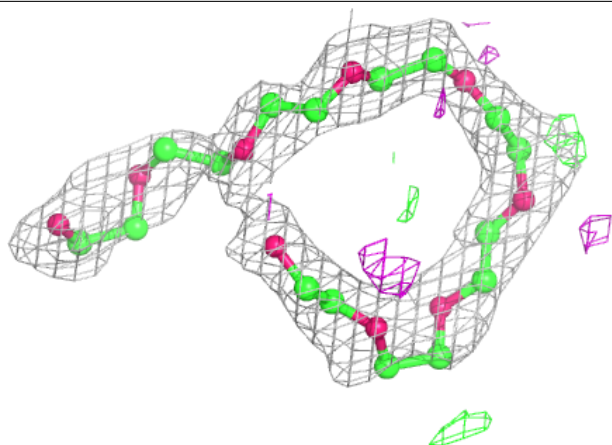
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

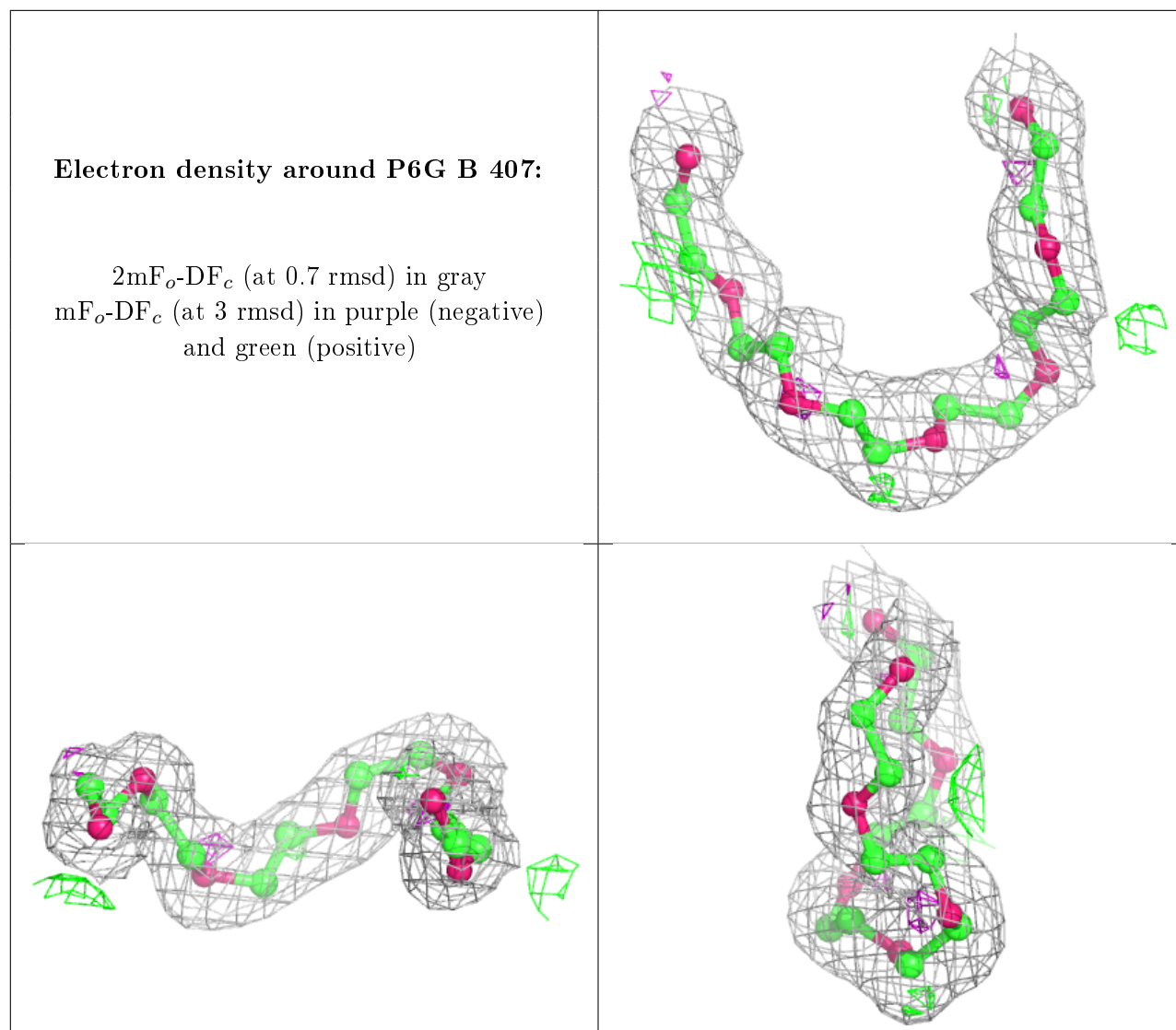
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	2PE	A	403	25/28	0.79	0.23	58,62,77,78	0
3	SO4	B	406	5/5	0.82	0.23	102,102,104,106	0
3	SO4	B	402	5/5	0.84	0.35	99,102,102,104	0
5	P6G	B	407	19/19	0.87	0.15	33,45,53,54	0
6	PG4	C	501	13/13	0.87	0.13	47,56,67,69	0
3	SO4	B	405	5/5	0.92	0.17	73,73,74,80	0
3	SO4	B	403	5/5	0.93	0.20	63,63,66,68	0
3	SO4	A	402	5/5	0.94	0.20	98,100,101,102	0
3	SO4	A	401	5/5	0.95	0.15	51,52,65,70	0
3	SO4	B	404	5/5	0.97	0.17	46,55,60,64	0
3	SO4	B	401	5/5	0.99	0.06	25,25,29,29	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 2PE A 403:**

$2mF_o-DF_c$  (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.