



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:39 AM UTC

PDB ID : 6KM7 / pdb_00006km7
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

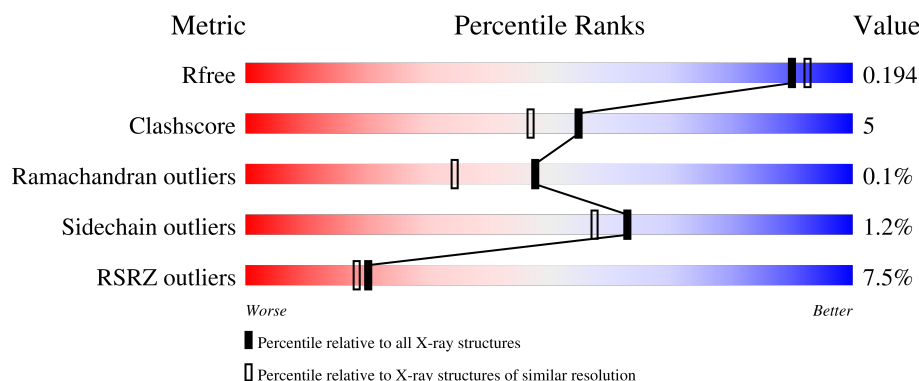
1 Overall quality at a glance

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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	A	317	5% 92% 7%
1	B	317	4% 88% 10%
2	C	69	7% 43% 54%
2	D	69	23% 43% 6% 51%

2 Entry composition

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
1	A	313	Total	C	N	O	S	0	0	0
			2439	1540	431	453	15			
1	B	312	Total	C	N	O	S	0	0	0
			2431	1536	429	451	15			

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
2	C	32	Total	C	N	O	0	1	0
			251	164	41	46			
2	D	34	Total	C	N	O	0	0	0
			266	175	45	46			

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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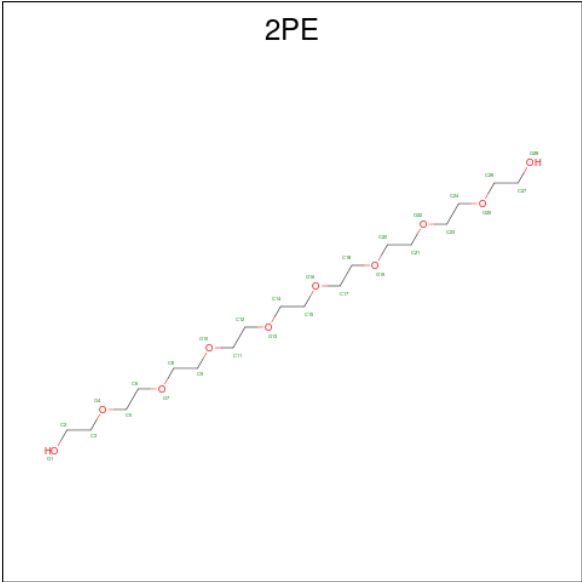
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP Q15291
C	?	-	ALA	deletion	UNP Q15291
C	?	-	SER	deletion	UNP Q15291
C	?	-	SER	deletion	UNP Q15291
C	?	-	GLU	deletion	UNP Q15291
C	?	-	LYS	deletion	UNP Q15291
C	?	-	LYS	deletion	UNP Q15291
C	?	-	ARG	deletion	UNP Q15291
C	?	-	GLN	deletion	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 (CCD ID: SO4) (formula: O₄S).



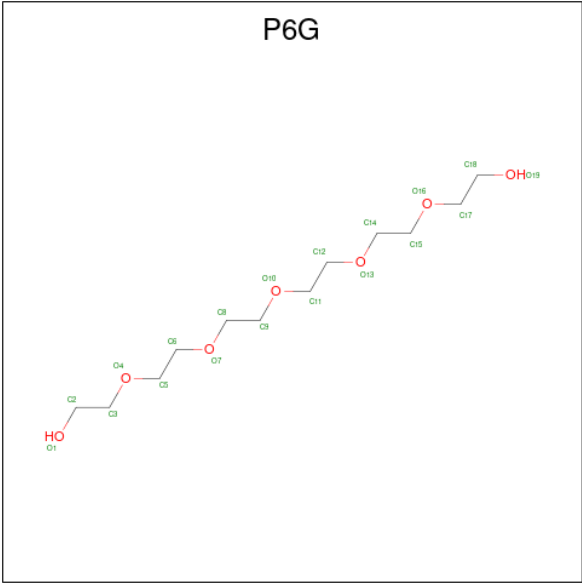
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



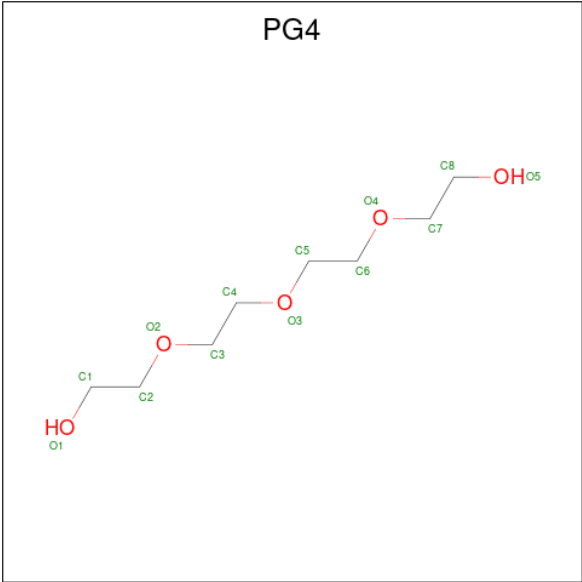
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			25	16	9		

- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

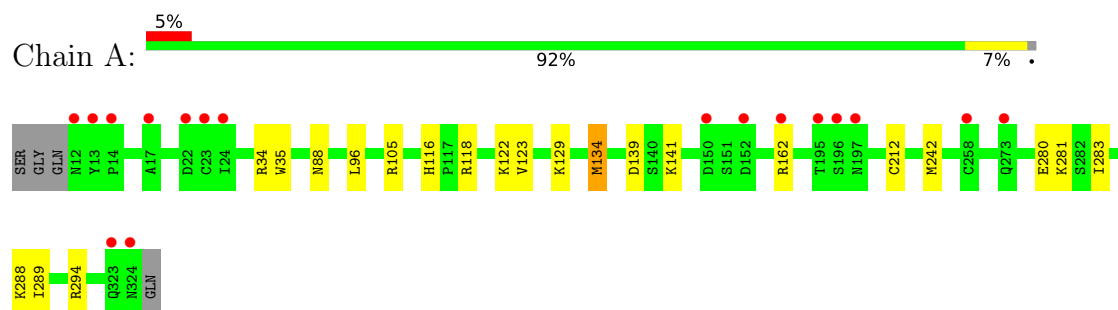
- Molecule 7 is water.

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		

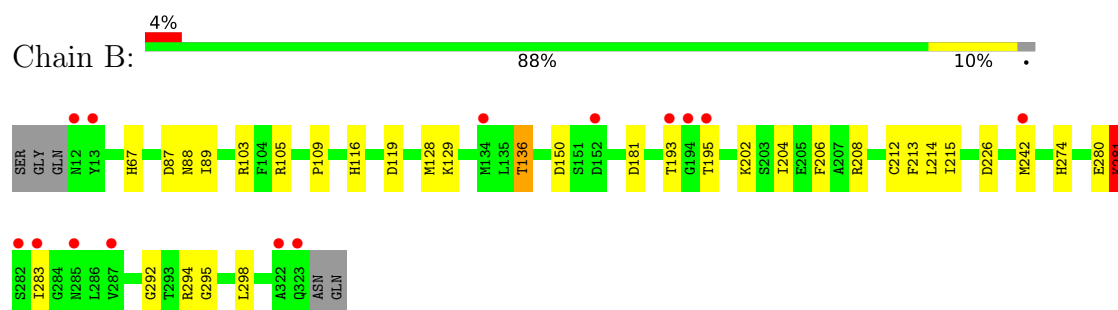
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

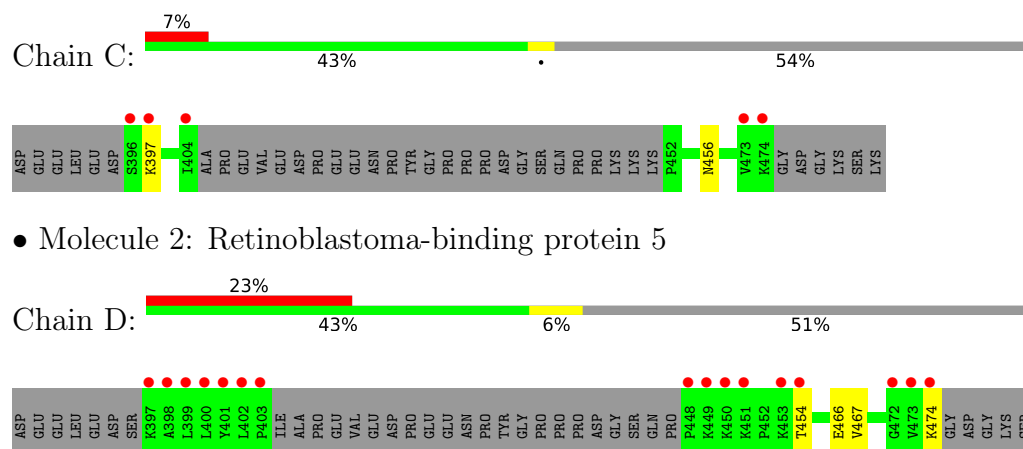
• Molecule 1: Retinoblastoma-binding protein 5



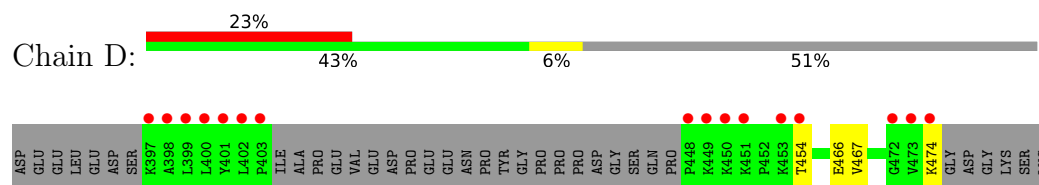
• Molecule 1: Retinoblastoma-binding protein 5



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.165 , 0.194 0.166 , 0.194	Depositor DCC
R_{free} test set	4355 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5963	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage'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.*

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: P6G, 2PE, PG4, SO4

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	0.44	2/2491 (0.1%)	0.58	0/3384
1	B	0.65	2/2483 (0.1%)	0.64	1/3373 (0.0%)
2	C	0.26	0/258	0.55	0/350
2	D	0.24	0/271	0.39	0/365
All	All	0.54	4/5503 (0.1%)	0.59	1/7472 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	GLU	C-O	-7.03	1.15	1.24
1	A	134	MET	SD-CE	-6.91	1.62	1.79
1	B	136	THR	C-O	-6.00	1.17	1.24
1	A	289	ILE	C-O	-5.09	1.18	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	LYS	N-CA-C	6.25	117.89	111.14

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	24	0
2	C	251	0	269	2	0
2	D	266	0	293	5	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
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	53	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 5.

All (53) 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:242:MET:HE1	1:A:281:LYS:HZ3	1.08	1.12
1:A:122:LYS:HB3	1:A:134:MET:HE2	1.30	1.10
1:A:116:HIS:HD2	1:A:118:ARG:H	1.27	0.83
1:A:242:MET:HE1	1:A:281:LYS:NZ	1.93	0.80
1:A:122:LYS:HB3	1:A:134:MET:CE	2.11	0.80
1:A:212:CYS:SG	1:A:281:LYS:NZ	2.56	0.75
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:B:128:MET:HE3	2:D:466:GLU:HB3	1.78	0.64
1:A:116:HIS:CD2	1:A:118:ARG:H	2.14	0.63
1:B:109:PRO:HB2	1:B:128:MET:HE2	1.82	0.61
1:B:294:ARG:HD3	1:B:295:GLY:N	2.15	0.61
1:A:35:TRP:CD1	4:A:403:2PE:H122	2.37	0.60
1:A:122:LYS:CB	1:A:134:MET:HE2	2.21	0.58
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:226:ASP:HB2	1:B:242:MET:HE1	1.89	0.53
1:A:123:VAL:N	1:A:134:MET:HE3	2.22	0.53
1:B:202:LYS:NZ	7:B:504:HOH:O	2.41	0.53
1:B:109:PRO:CG	1:B:128:MET:HE2	2.40	0.52
1:A:139:ASP:CG	1:A:141:LYS:HD3	2.37	0.50
1:B:109:PRO:CB	1:B:128:MET:HE2	2.43	0.49
2:D:474:LYS:HG3	2:D:474:LYS:O	2.13	0.48
1:A:35:TRP:NE1	4:A:403:2PE:H82	2.29	0.47
1:B:128:MET:HE1	2:D:467:VAL:O	2.15	0.47
5:B:407:P6G:H171	7:B:665:HOH:O	2.14	0.47
1:A:280:GLU:OE2	1:A:283:ILE:HD12	2.15	0.47
1:B:128:MET:CE	2:D:466:GLU:HB3	2.43	0.46
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: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:HD2	2:C:397:LYS:HA	1.53	0.43
5:B:407:P6G:H111	5:B:407:P6G:H141	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:A:123:VAL:N	1:A:134:MET:CE	2.84	0.41
1:B:214:LEU:C	1:B:214:LEU:HD12	2.46	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

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	311/317 (98%)	304 (98%)	6 (2%)	1 (0%)	36	25
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%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ASN

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	272/275 (99%)	270 (99%)	2 (1%)	76	73
1	B	271/275 (98%)	266 (98%)	5 (2%)	51	43
2	C	30/61 (49%)	30 (100%)	0	100	100
2	D	31/61 (51%)	31 (100%)	0	100	100
All	All	604/672 (90%)	597 (99%)	7 (1%)	63	57

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	288	LYS
1	B	88	ASN
1	B	150	ASP
1	B	281	LYS

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Mol	Chain	Res	Type
1	B	283	ILE
1	B	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	142	HIS
1	A	246	GLN
1	A	323	GLN
1	B	246	GLN
1	B	274	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 oligosaccharides 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	$\# Z > 2$
5	P6G	B	407	-	18,18,18	0.54	0	17,17,17	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	402	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	402	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	B	404	-	4,4,4	0.21	0	6,6,6	0.14	0
6	PG4	C	501	-	12,12,12	0.55	0	11,11,11	0.33	0
3	SO4	B	406	-	4,4,4	0.24	0	6,6,6	0.12	0
4	2PE	A	403	-	24,24,27	0.55	0	23,23,26	0.30	0
3	SO4	A	401	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	B	403	-	4,4,4	0.21	0	6,6,6	0.18	0
3	SO4	B	405	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	B	401	-	4,4,4	0.21	0	6,6,6	0.33	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	-
6	PG4	C	501	-	-	6/10/10/10	-
5	P6G	B	407	-	-	9/16/16/16	-

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

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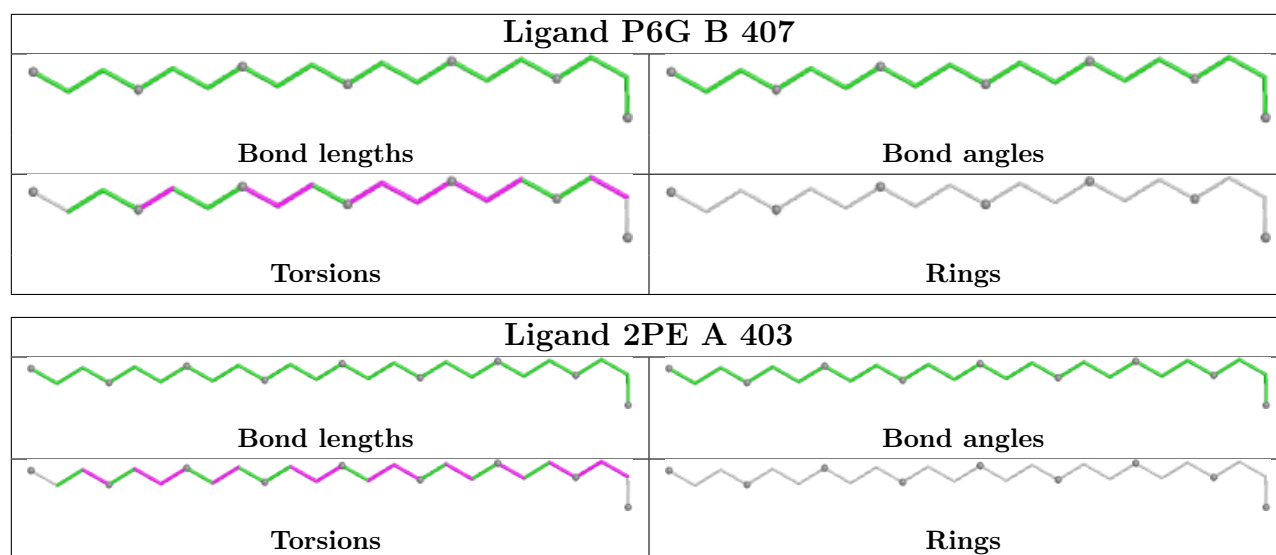
Mol	Chain	Res	Type	Atoms
4	A	403	2PE	C6-C5-O4-C3
5	B	407	P6G	C5-C6-O7-C8
4	A	403	2PE	O13-C14-C15-O16
4	A	403	2PE	C5-C6-O7-C8
6	C	501	PG4	C3-C4-O3-C5
4	A	403	2PE	C15-C14-O13-C12
6	C	501	PG4	C8-C7-O4-C6
4	A	403	2PE	C12-C11-O10-C9
4	A	403	2PE	O16-C17-C18-O19
4	A	403	2PE	O7-C8-C9-O10
5	B	407	P6G	C9-C8-O7-C6
5	B	407	P6G	C8-C9-O10-C11
4	A	403	2PE	C21-C20-O19-C18
4	A	403	2PE	C2-C3-O4-C5
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
5	B	407	P6G	3	0
6	C	501	PG4	1	0
4	A	403	2PE	6	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 ⓘ

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, 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	A	313/317 (98%)	-0.14	17 (5%) 31 30	14, 24, 53, 90	0
1	B	312/317 (98%)	-0.07	14 (4%) 38 37	14, 26, 55, 95	0
2	C	32/69 (46%)	0.79	5 (15%) 5 4	20, 35, 61, 96	1 (3%)
2	D	34/69 (49%)	2.06	16 (47%) 0 0	28, 53, 96, 101	0
All	All	691/772 (89%)	0.05	52 (7%) 20 18	14, 26, 60, 101	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	448	PRO	7.4
2	D	401	TYR	5.6
2	D	403	PRO	5.4
2	D	473	VAL	5.2
1	B	195	THR	4.5
2	D	402	LEU	4.4
2	C	404	ILE	4.3
1	A	195	THR	4.2
1	B	13	TYR	4.1
1	A	324	ASN	3.9
1	A	196	SER	3.7
1	B	282	SER	3.6
1	A	323	GLN	3.4
1	B	12	ASN	3.3
2	D	399	LEU	3.2
2	D	472	GLY	3.2
2	D	450	LYS	3.2
2	D	398	ALA	3.2
1	B	283	ILE	3.2
1	A	13	TYR	3.2
2	D	474	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	152	ASP	3.2
1	A	22	ASP	3.1
2	C	397	LYS	3.1
2	D	449	LYS	3.1
2	D	451	LYS	3.0
1	B	194	GLY	2.8
2	C	473	VAL	2.8
2	C	396	SER	2.7
1	B	287	VAL	2.7
1	B	285	ASN	2.7
1	A	14	PRO	2.7
1	B	322	ALA	2.6
1	A	152	ASP	2.6
1	B	323	GLN	2.6
2	D	397	LYS	2.6
1	A	12	ASN	2.6
1	A	17	ALA	2.6
1	A	273	GLN	2.5
1	B	193	THR	2.5
2	D	400	LEU	2.5
1	A	258	CYS	2.5
2	D	454	THR	2.4
1	A	150	ASP	2.4
1	A	24	ILE	2.4
1	A	197	ASN	2.4
1	A	23	CYS	2.3
1	A	162	ARG	2.3
1	B	134	MET	2.3
1	B	242	MET	2.3
2	C	474	LYS	2.2
2	D	453	LYS	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 oligosaccharides in this entry.

6.4 Ligands

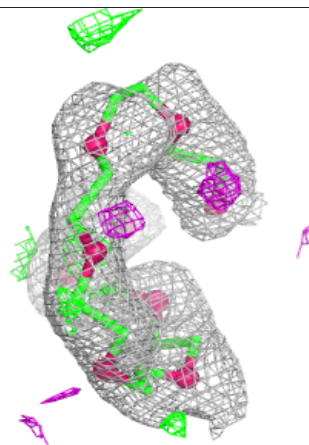
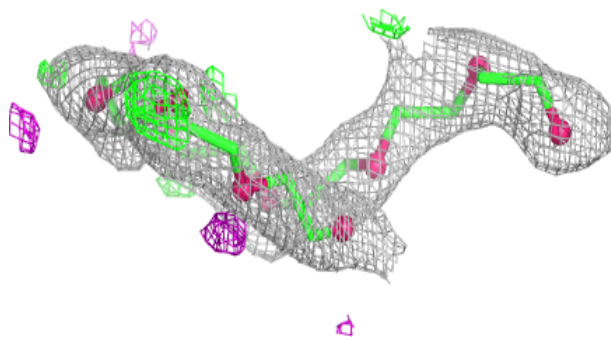
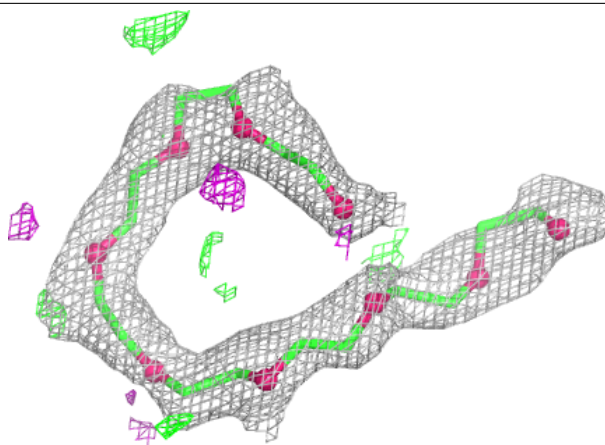
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	402	5/5	0.70	0.14	99,102,102,104	0
3	SO4	B	406	5/5	0.79	0.14	102,102,104,106	0
4	2PE	A	403	25/28	0.84	0.18	58,62,77,78	0
3	SO4	A	402	5/5	0.85	0.12	98,100,101,102	0
3	SO4	B	403	5/5	0.85	0.12	63,63,66,68	0
3	SO4	A	401	5/5	0.88	0.11	51,52,65,70	0
6	PG4	C	501	13/13	0.88	0.15	47,56,67,69	0
3	SO4	B	405	5/5	0.89	0.12	73,73,74,80	0
5	P6G	B	407	19/19	0.91	0.12	33,45,53,54	0
3	SO4	B	404	5/5	0.94	0.09	46,55,60,64	0
3	SO4	B	401	5/5	0.99	0.04	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.

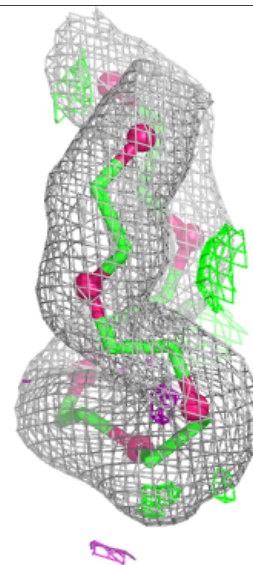
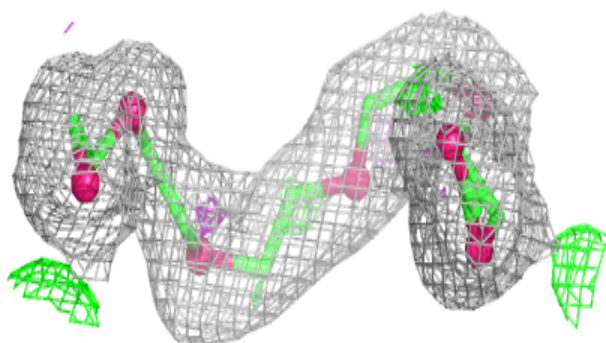
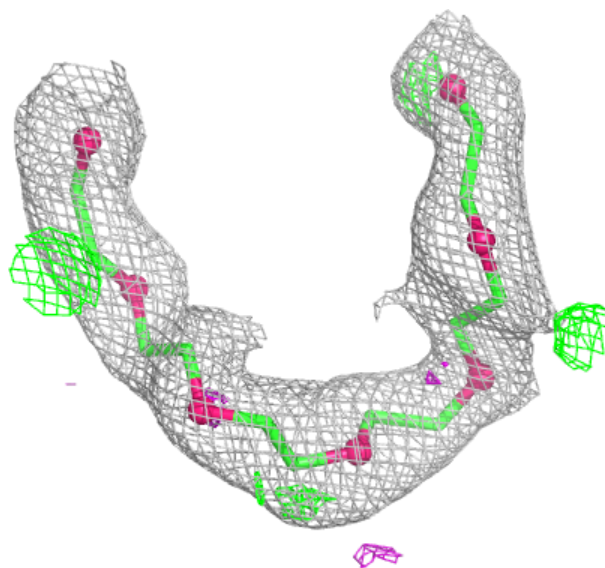
Electron density around 2PE A 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P6G B 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.