



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2025 – 09:02 am BST

PDB ID : 9RM2 / pdb_00009rm2
Title : BKP_yV VP1 IN COMPLEX WITH 319C07-FAB
Authors : Schmitt, S.; Hillenbrand, M.
Deposited on : 2025-06-17
Resolution : 1.96 Å(reported)

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 ⓘ 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

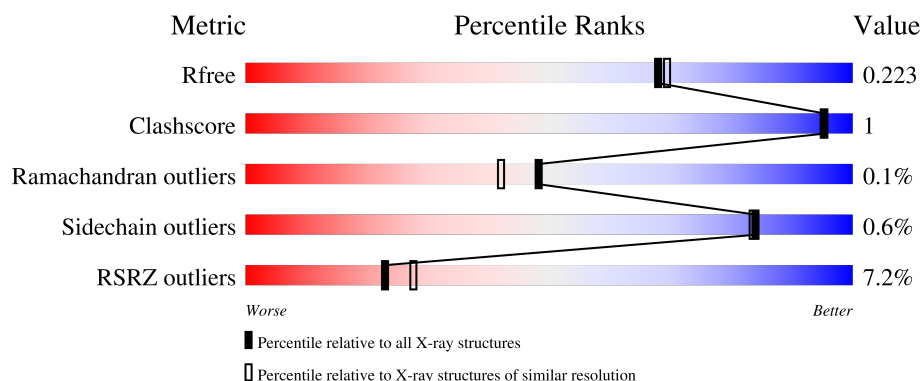
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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	223	<div> <div>7%</div> <div>96%</div> </div>
1	D	223	<div> <div>10%</div> <div>98%</div> </div>
1	G	223	<div> <div>6%</div> <div>96%</div> </div>
1	H	223	<div> <div>16%</div> <div>96%</div> </div>
1	M	223	<div> <div>4%</div> <div>98%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	215	
2	E	215	
2	J	215	
2	L	215	
2	N	215	
3	C	300	
3	F	300	
3	K	300	
3	O	300	
3	P	300	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 29832 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 319C07 antibody heavy chain, Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	215	Total	C	N	O	S	54	0	0
			1656	1059	279	314	4			
1	A	218	Total	C	N	O	S	31	1	0
			1685	1076	286	319	4			
1	D	223	Total	C	N	O	S	46	1	0
			1713	1093	289	327	4			
1	G	222	Total	C	N	O	S	26	3	0
			1719	1096	292	327	4			
1	M	222	Total	C	N	O	S	17	2	0
			1709	1090	288	327	4			

- Molecule 2 is a protein called 319C07 antibody light chain, Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	49	3	0
			1638	1027	276	331	4			
2	B	215	Total	C	N	O	S	30	1	0
			1641	1028	275	333	5			
2	E	212	Total	C	N	O	S	64	0	0
			1619	1016	272	327	4			
2	J	214	Total	C	N	O	S	22	0	0
			1632	1023	274	331	4			
2	N	214	Total	C	N	O	S	16	0	0
			1632	1023	274	331	4			

- Molecule 3 is a protein called Major capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	274	Total	C	N	O	S	21	8	0
			2170	1364	375	418	13			
3	C	268	Total	C	N	O	S	16	5	0
			2115	1327	374	402	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	267	Total	C	N	O	S	21	4	0
			2094	1316	364	402	12			
3	K	273	Total	C	N	O	S	12	2	0
			2127	1336	369	410	12			
3	O	273	Total	C	N	O	S	17	3	0
			2135	1341	372	410	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	80	SER	CYS	engineered mutation	UNP P03088
P	133	ASP	GLU	variant	UNP P03088
P	146	THR	SER	variant	UNP P03088
P	194	THR	ALA	variant	UNP P03088
C	80	SER	CYS	engineered mutation	UNP P03088
C	133	ASP	GLU	variant	UNP P03088
C	146	THR	SER	variant	UNP P03088
C	194	THR	ALA	variant	UNP P03088
F	80	SER	CYS	engineered mutation	UNP P03088
F	133	ASP	GLU	variant	UNP P03088
F	146	THR	SER	variant	UNP P03088
F	194	THR	ALA	variant	UNP P03088
K	80	SER	CYS	engineered mutation	UNP P03088
K	133	ASP	GLU	variant	UNP P03088
K	146	THR	SER	variant	UNP P03088
K	194	THR	ALA	variant	UNP P03088
O	80	SER	CYS	engineered mutation	UNP P03088
O	133	ASP	GLU	variant	UNP P03088
O	146	THR	SER	variant	UNP P03088
O	194	THR	ALA	variant	UNP P03088

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

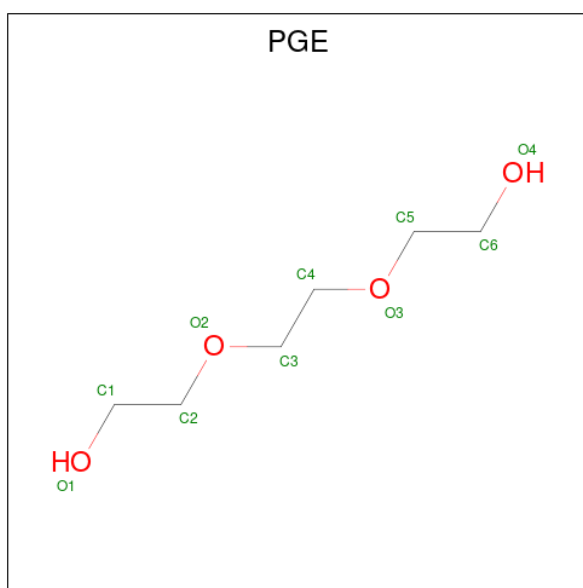
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Cl	0	0
			1	1		
4	P	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	K	1	Total	Cl	0	0
			1	1		
4	M	1	Total	Cl	0	0
			1	1		
4	O	1	Total	Cl	0	0
			1	1		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



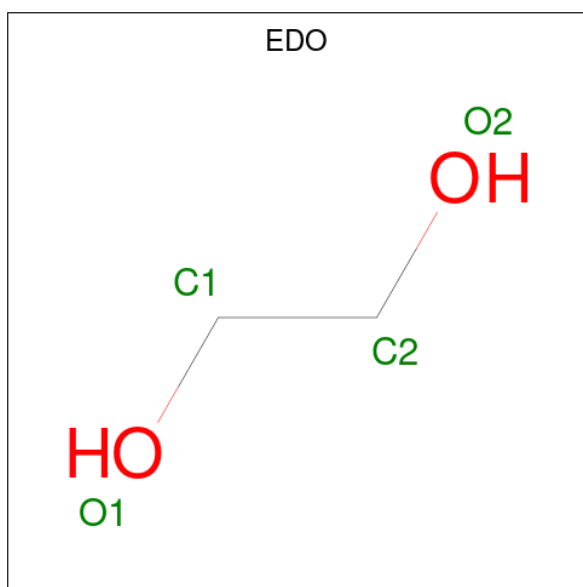
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			10	6	4		
5	H	1	Total	C	O	0	0
			10	6	4		
5	P	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		
5	M	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



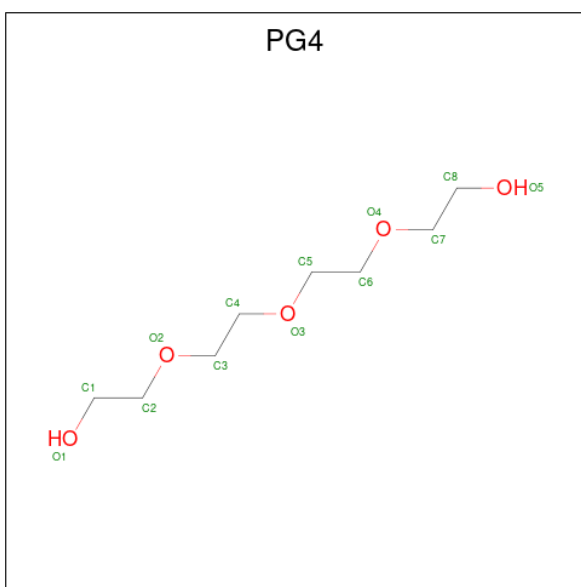
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	P	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

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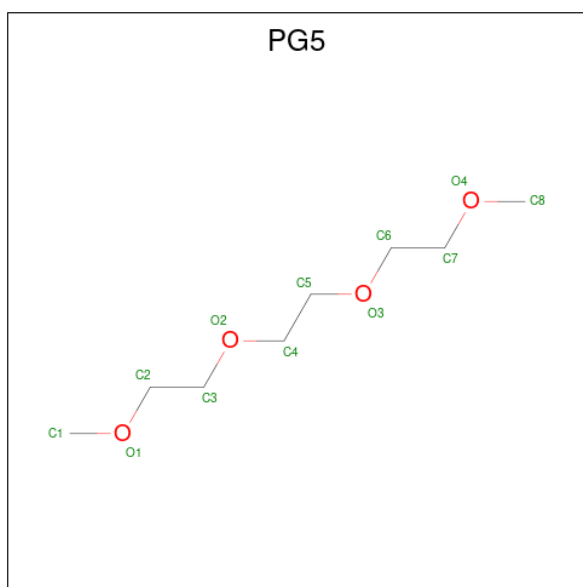
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	J	1	Total 4	C 2	O 2	0	0
6	J	1	Total 4	C 2	O 2	0	0
6	K	1	Total 4	C 2	O 2	0	0
6	K	1	Total 4	C 2	O 2	0	0
6	K	1	Total 4	C 2	O 2	0	0
6	K	1	Total 4	C 2	O 2	0	0
6	K	1	Total 4	C 2	O 2	0	0
6	M	1	Total 4	C 2	O 2	0	0
6	M	1	Total 4	C 2	O 2	0	0
6	M	1	Total 4	C 2	O 2	0	0
6	M	1	Total 4	C 2	O 2	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



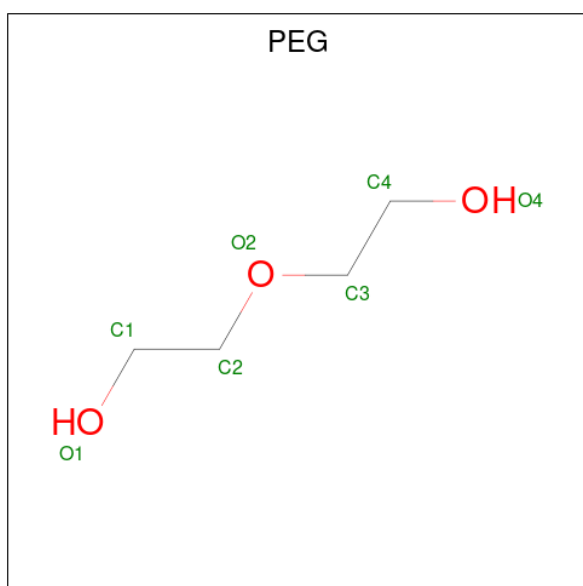
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			13	8	5		
7	P	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	M	1	Total	C	O	0	0
			13	8	5		
7	N	1	Total	C	O	0	0
			13	8	5		
7	N	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (CCD ID: PG5) (formula: C₈H₁₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			12	8	4		
8	J	1	Total	C	O	0	0
			12	8	4		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



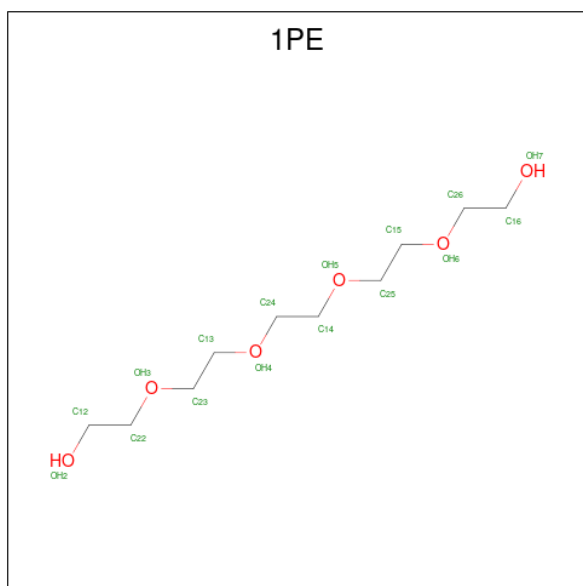
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		

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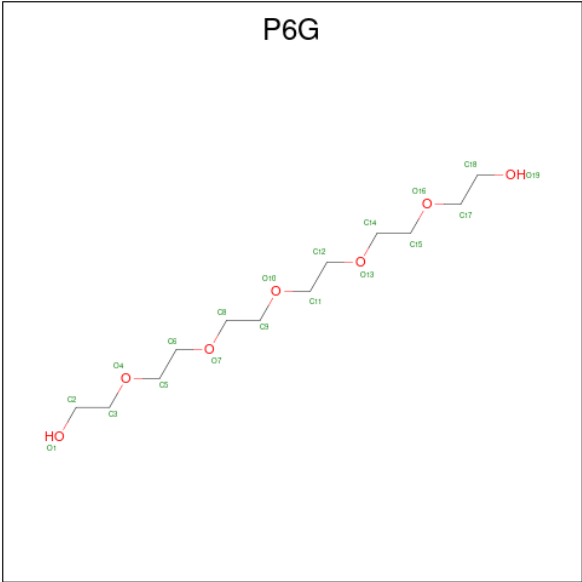
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			7	4	3		
9	F	1	Total	C	O	0	0
			7	4	3		
9	K	1	Total	C	O	0	0
			7	4	3		
9	K	1	Total	C	O	0	0
			7	4	3		
9	N	1	Total	C	O	0	0
			7	4	3		
9	O	1	Total	C	O	0	0
			7	4	3		
9	O	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	0
			16	10	6		

- Molecule 11 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



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

- Molecule 12 is water.

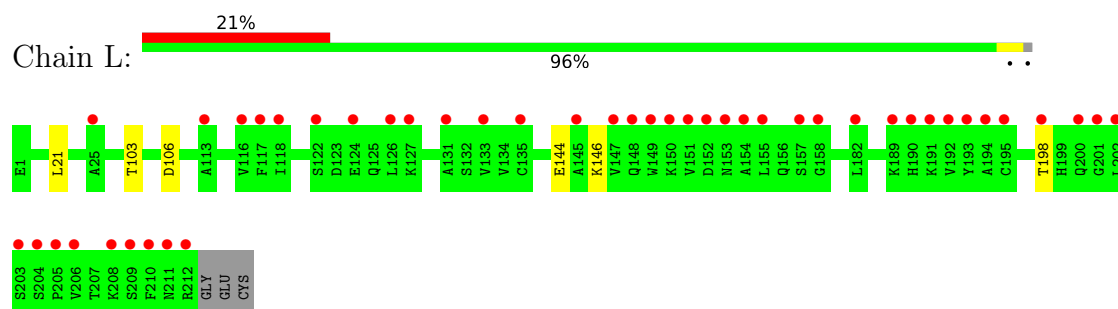
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	89	Total	O	0	0
			89	89		
12	L	80	Total	O	0	0
			80	80		
12	P	198	Total	O	0	0
			198	198		
12	A	108	Total	O	0	0
			108	108		
12	B	153	Total	O	0	0
			153	153		
12	C	173	Total	O	0	0
			173	173		
12	D	76	Total	O	0	0
			76	76		
12	E	96	Total	O	0	0
			96	96		
12	F	173	Total	O	0	0
			173	173		
12	G	153	Total	O	0	0
			153	153		
12	J	143	Total	O	0	0
			143	143		

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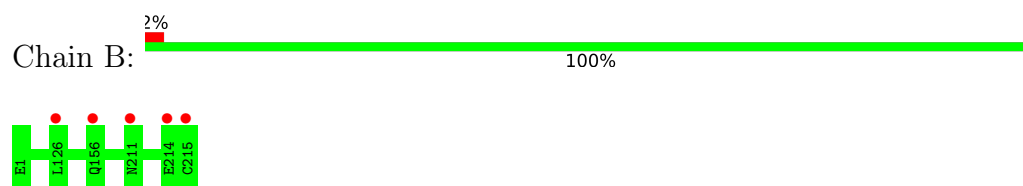
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	K	222	Total 222	O 222	0	0
12	M	124	Total 124	O 124	0	0
12	N	162	Total 162	O 162	0	0
12	O	206	Total 206	O 206	0	0

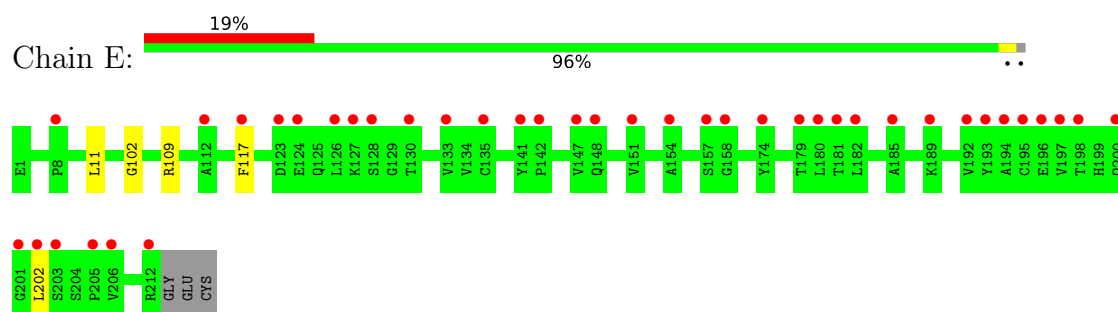
- Molecule 2: 319C07 antibody light chain, Fab fragment



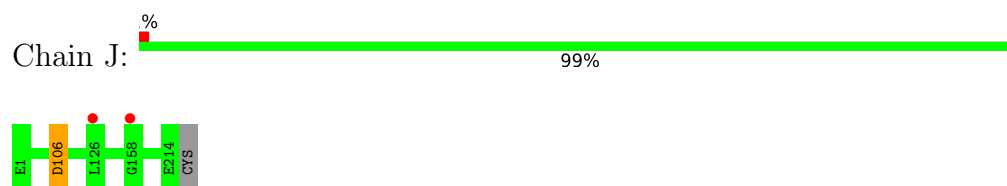
- Molecule 2: 319C07 antibody light chain, Fab fragment



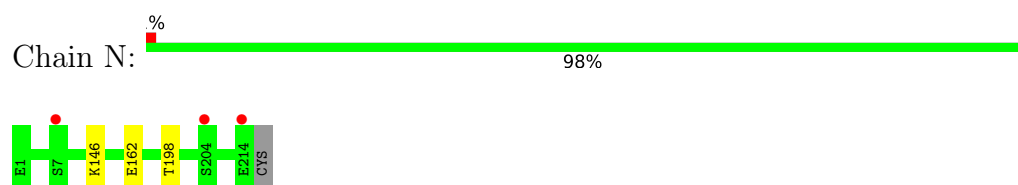
- Molecule 2: 319C07 antibody light chain, Fab fragment



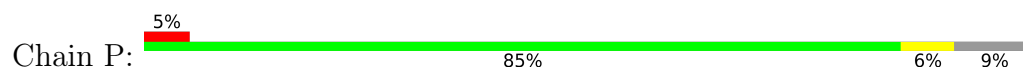
- Molecule 2: 319C07 antibody light chain, Fab fragment

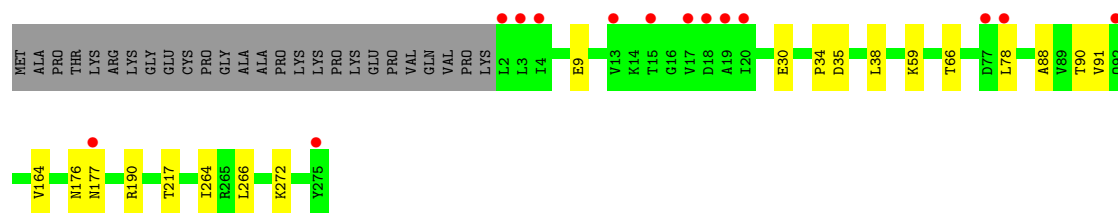


- Molecule 2: 319C07 antibody light chain, Fab fragment

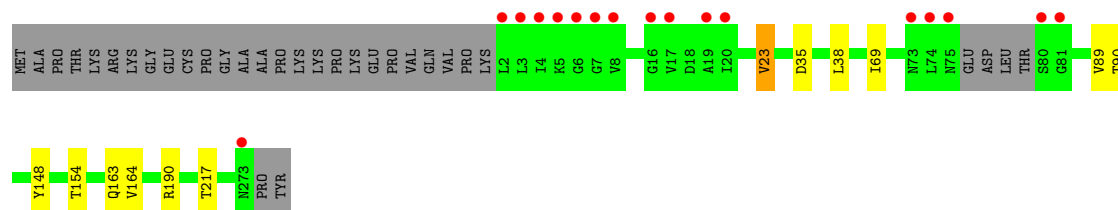
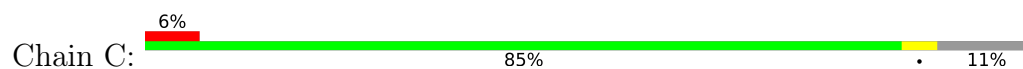


- Molecule 3: Major capsid protein VP1

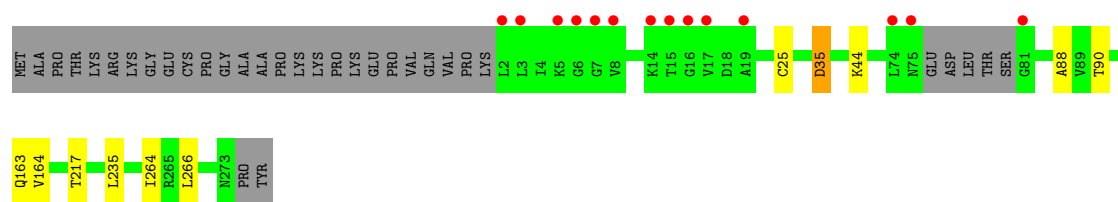
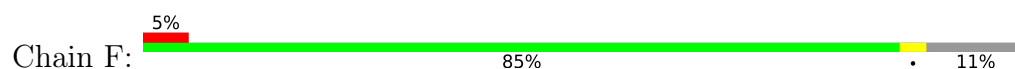




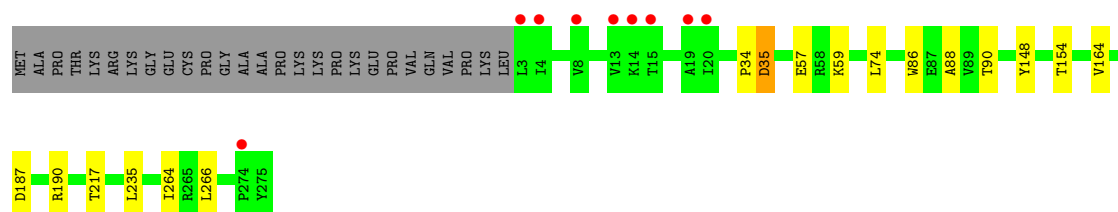
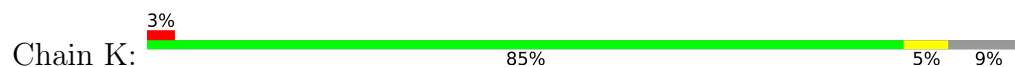
• Molecule 3: Major capsid protein VP1



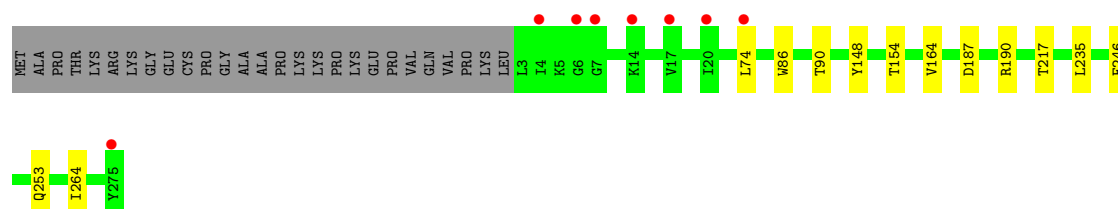
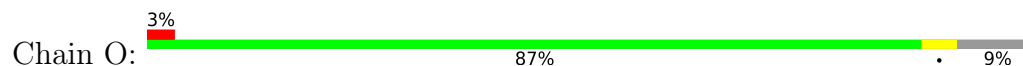
• Molecule 3: Major capsid protein VP1



• Molecule 3: Major capsid protein VP1



• Molecule 3: Major capsid protein VP1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.35Å 172.08Å 113.14Å 90.00° 97.64° 90.00°	Depositor
Resolution (Å)	91.87 – 1.96 91.87 – 1.96	Depositor EDS
% Data completeness (in resolution range)	92.5 (91.87-1.96) 92.6 (91.87-1.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.187 , 0.218 0.193 , 0.223	Depositor DCC
R_{free} test set	14637 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29832	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG5, PEG, P6G, PGE, EDO, 1PE, PG4, CL

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	1.00	0/1736	1.27	0/2369
1	D	1.03	0/1765	1.25	1/2410 (0.0%)
1	G	1.01	0/1777	1.25	0/2425
1	H	1.01	0/1704	1.26	1/2328 (0.0%)
1	M	1.00	0/1764	1.25	1/2408 (0.0%)
2	B	1.01	0/1680	1.27	0/2285
2	E	1.03	0/1655	1.28	3/2251 (0.1%)
2	J	1.01	0/1668	1.28	1/2268 (0.0%)
2	L	1.04	0/1680	1.27	0/2284
2	N	1.01	0/1668	1.27	0/2268
3	C	0.99	0/2166	1.23	0/2936
3	F	0.98	0/2145	1.23	1/2910 (0.0%)
3	K	0.97	0/2181	1.24	1/2963 (0.0%)
3	O	0.98	0/2192	1.23	0/2977
3	P	1.00	0/2236	1.24	0/3036
All	All	1.00	0/28017	1.25	9/38118 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	35	ASP	CA-CB-CG	7.48	120.08	112.60
3	F	35	ASP	CA-CB-CG	6.76	119.36	112.60
1	M	27	GLY	CA-C-O	-5.88	118.17	122.23
2	J	106	ASP	CA-CB-CG	5.78	118.38	112.60
1	D	27	GLY	CA-C-O	-5.50	118.44	122.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1685	0	1651	2	0
1	D	1713	0	1681	2	0
1	G	1719	0	1691	2	0
1	H	1656	0	1615	0	0
1	M	1709	0	1677	2	0
2	B	1641	0	1601	0	0
2	E	1619	0	1582	1	0
2	J	1632	0	1591	0	0
2	L	1638	0	1603	3	0
2	N	1632	0	1591	2	0
3	C	2115	0	2088	12	0
3	F	2094	0	2060	6	0
3	K	2127	0	2088	8	0
3	O	2135	0	2101	7	0
3	P	2170	0	2139	13	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	B	30	0	42	0	0
5	C	10	0	14	0	0
5	E	10	0	14	0	0
5	H	20	0	28	0	0
5	M	10	0	14	0	0
5	P	10	0	14	0	0
6	B	8	0	12	0	0
6	C	8	0	12	0	0
6	D	12	0	18	0	0
6	F	4	0	6	0	0
6	G	4	0	6	0	0
6	H	8	0	12	0	0
6	J	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	20	0	30	0	0
6	M	16	0	24	0	0
6	P	4	0	6	0	0
7	B	13	0	18	0	0
7	L	13	0	18	0	0
7	M	13	0	18	0	0
7	N	26	0	36	0	0
7	P	13	0	18	0	0
8	J	12	0	18	0	0
8	L	12	0	18	0	0
9	B	7	0	10	0	0
9	D	7	0	10	0	0
9	E	7	0	10	0	0
9	F	7	0	10	0	0
9	K	14	0	20	0	0
9	N	7	0	10	0	0
9	O	14	0	20	0	0
10	G	16	0	22	0	0
11	J	19	0	26	0	0
12	A	108	0	0	1	0
12	B	153	0	0	0	0
12	C	173	0	0	0	0
12	D	76	0	0	0	0
12	E	96	0	0	1	0
12	F	173	0	0	1	0
12	G	153	0	0	0	0
12	H	89	0	0	0	0
12	J	143	0	0	0	0
12	K	222	0	0	1	0
12	L	80	0	0	0	0
12	M	124	0	0	0	0
12	N	162	0	0	2	0
12	O	206	0	0	1	0
12	P	198	0	0	1	0
All	All	29832	0	27305	57	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 1.

The worst 5 of 57 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)
3:C:190[B]:ARG:HH11	3:C:190[B]:ARG:CG	1.87	0.88
3:F:25:CYS:SG	12:F:558:HOH:O	2.32	0.86
3:C:190[B]:ARG:HH11	3:C:190[B]:ARG:HG3	1.45	0.80
1:M:58:ASN:HB3	12:N:401:HOH:O	1.87	0.74
3:F:235:LEU:HD21	3:F:264:ILE:HD13	1.75	0.68

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	215/223 (96%)	212 (99%)	3 (1%)	0	100	100
1	D	222/223 (100%)	219 (99%)	3 (1%)	0	100	100
1	G	223/223 (100%)	220 (99%)	3 (1%)	0	100	100
1	H	211/223 (95%)	208 (99%)	3 (1%)	0	100	100
1	M	222/223 (100%)	219 (99%)	3 (1%)	0	100	100
2	B	214/215 (100%)	208 (97%)	6 (3%)	0	100	100
2	E	210/215 (98%)	203 (97%)	7 (3%)	0	100	100
2	J	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
2	L	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
2	N	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
3	C	269/300 (90%)	258 (96%)	10 (4%)	1 (0%)	30	21
3	F	267/300 (89%)	255 (96%)	11 (4%)	1 (0%)	30	21
3	K	273/300 (91%)	261 (96%)	11 (4%)	1 (0%)	30	21
3	O	274/300 (91%)	263 (96%)	10 (4%)	1 (0%)	30	21
3	P	280/300 (93%)	267 (95%)	12 (4%)	1 (0%)	30	21
All	All	3517/3690 (95%)	3416 (97%)	96 (3%)	5 (0%)	48	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	164	VAL
3	F	164	VAL
3	K	164	VAL
3	O	164	VAL
3	P	164	VAL

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	188/191 (98%)	186 (99%)	2 (1%)	70	68
1	D	192/191 (100%)	192 (100%)	0	100	100
1	G	193/191 (101%)	190 (98%)	3 (2%)	58	55
1	H	184/191 (96%)	183 (100%)	1 (0%)	86	86
1	M	192/191 (100%)	191 (100%)	1 (0%)	86	86
2	B	188/187 (100%)	188 (100%)	0	100	100
2	E	185/187 (99%)	183 (99%)	2 (1%)	70	68
2	J	186/187 (100%)	185 (100%)	1 (0%)	86	86
2	L	188/187 (100%)	187 (100%)	1 (0%)	86	86
2	N	186/187 (100%)	186 (100%)	0	100	100
3	C	235/257 (91%)	233 (99%)	2 (1%)	75	75
3	F	233/257 (91%)	232 (100%)	1 (0%)	89	89
3	K	237/257 (92%)	235 (99%)	2 (1%)	79	78
3	O	238/257 (93%)	238 (100%)	0	100	100
3	P	244/257 (95%)	242 (99%)	2 (1%)	79	78
All	All	3069/3175 (97%)	3051 (99%)	18 (1%)	84	83

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	106	ASP
1	M	217	LYS
3	K	57	GLU
2	E	11	LEU
1	G	146	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	138	ASN
2	J	138	ASN
2	N	138	ASN
1	G	53	HIS
2	J	139	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 9 are monoatomic - leaving 51 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	C	304	-	3,3,3	0.16	0	2,2,2	0.45	0
6	EDO	J	302	-	3,3,3	0.10	0	2,2,2	0.29	0
9	PEG	K	302	-	6,6,6	0.18	0	5,5,5	0.20	0
6	EDO	P	304	-	3,3,3	0.17	0	2,2,2	0.46	0
6	EDO	K	308	-	3,3,3	0.13	0	2,2,2	0.45	0
9	PEG	B	305	-	6,6,6	0.17	0	5,5,5	0.10	0
5	PGE	H	302	-	9,9,9	0.14	0	8,8,8	0.16	0
5	PGE	B	303	-	9,9,9	0.21	0	8,8,8	0.18	0
6	EDO	K	306	-	3,3,3	0.10	0	2,2,2	0.30	0
11	P6G	J	304	-	18,18,18	0.24	0	17,17,17	0.27	0
6	EDO	B	306	-	3,3,3	0.13	0	2,2,2	0.37	0
7	PG4	N	302	-	12,12,12	0.21	0	11,11,11	0.22	0
9	PEG	O	302	-	6,6,6	0.16	0	5,5,5	0.17	0
10	1PE	G	301	-	15,15,15	0.21	0	14,14,14	0.24	0
6	EDO	B	307	-	3,3,3	0.16	0	2,2,2	0.44	0
6	EDO	H	305	-	3,3,3	0.10	0	2,2,2	0.27	0
8	PG5	J	301	-	11,11,11	0.22	0	10,10,10	0.23	0
5	PGE	H	303	-	9,9,9	0.20	0	8,8,8	0.16	0
6	EDO	K	307	-	3,3,3	0.08	0	2,2,2	0.34	0
7	PG4	B	301	-	12,12,12	0.23	0	11,11,11	0.16	0
6	EDO	F	302	-	3,3,3	0.16	0	2,2,2	0.49	0
6	EDO	M	304	-	3,3,3	0.13	0	2,2,2	0.33	0
6	EDO	K	304	-	3,3,3	0.13	0	2,2,2	0.38	0
7	PG4	N	301	-	12,12,12	0.20	0	11,11,11	0.25	0
6	EDO	M	307	-	3,3,3	0.07	0	2,2,2	0.27	0
7	PG4	P	302	-	12,12,12	0.17	0	11,11,11	0.18	0
6	EDO	K	305	-	3,3,3	0.15	0	2,2,2	0.43	0
5	PGE	B	304	-	9,9,9	0.17	0	8,8,8	0.20	0
9	PEG	D	302	-	6,6,6	0.18	0	5,5,5	0.16	0
6	EDO	D	301	-	3,3,3	0.05	0	2,2,2	0.29	0
5	PGE	E	302	-	9,9,9	0.18	0	8,8,8	0.15	0
6	EDO	M	305	-	3,3,3	0.08	0	2,2,2	0.30	0
9	PEG	N	303	-	6,6,6	0.14	0	5,5,5	0.10	0
7	PG4	L	301	-	12,12,12	0.20	0	11,11,11	0.16	0
7	PG4	M	302	-	12,12,12	0.17	0	11,11,11	0.22	0
9	PEG	O	303	-	6,6,6	0.17	0	5,5,5	0.13	0
5	PGE	B	302	-	9,9,9	0.16	0	8,8,8	0.19	0
6	EDO	H	304	-	3,3,3	0.14	0	2,2,2	0.42	0
9	PEG	K	303	-	6,6,6	0.16	0	5,5,5	0.11	0
5	PGE	P	303	-	9,9,9	0.23	0	8,8,8	0.17	0
6	EDO	G	302	-	3,3,3	0.12	0	2,2,2	0.32	0
5	PGE	M	303	-	9,9,9	0.22	0	8,8,8	0.18	0
9	PEG	E	303	-	6,6,6	0.14	0	5,5,5	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PGE	C	302	-	9,9,9	0.18	0	8,8,8	0.14	0
6	EDO	J	303	-	3,3,3	0.17	0	2,2,2	0.32	0
9	PEG	F	303	-	6,6,6	0.23	0	5,5,5	0.19	0
8	PG5	L	302	-	11,11,11	0.19	0	10,10,10	0.18	0
6	EDO	C	303	-	3,3,3	0.11	0	2,2,2	0.38	0
6	EDO	M	306	-	3,3,3	0.11	0	2,2,2	0.29	0
6	EDO	D	303	-	3,3,3	0.08	0	2,2,2	0.30	0
6	EDO	D	304	-	3,3,3	0.09	0	2,2,2	0.30	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	C	304	-	-	1/1/1/1	-
6	EDO	J	302	-	-	0/1/1/1	-
9	PEG	K	302	-	-	3/4/4/4	-
6	EDO	P	304	-	-	1/1/1/1	-
6	EDO	K	308	-	-	1/1/1/1	-
9	PEG	B	305	-	-	1/4/4/4	-
5	PGE	H	302	-	-	3/7/7/7	-
5	PGE	B	303	-	-	3/7/7/7	-
6	EDO	K	306	-	-	1/1/1/1	-
11	P6G	J	304	-	-	6/16/16/16	-
6	EDO	B	306	-	-	1/1/1/1	-
7	PG4	N	302	-	-	5/10/10/10	-
9	PEG	O	302	-	-	3/4/4/4	-
10	1PE	G	301	-	-	2/13/13/13	-
6	EDO	B	307	-	-	1/1/1/1	-
6	EDO	H	305	-	-	1/1/1/1	-
8	PG5	J	301	-	-	2/9/9/9	-
5	PGE	H	303	-	-	4/7/7/7	-
6	EDO	K	307	-	-	1/1/1/1	-
7	PG4	B	301	-	-	2/10/10/10	-
6	EDO	F	302	-	-	1/1/1/1	-
6	EDO	M	304	-	-	0/1/1/1	-
6	EDO	K	304	-	-	1/1/1/1	-
7	PG4	N	301	-	-	7/10/10/10	-
6	EDO	M	307	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	P	302	-	-	2/10/10/10	-
6	EDO	K	305	-	-	1/1/1/1	-
5	PGE	B	304	-	-	1/7/7/7	-
9	PEG	D	302	-	-	2/4/4/4	-
6	EDO	D	301	-	-	1/1/1/1	-
5	PGE	E	302	-	-	3/7/7/7	-
6	EDO	M	305	-	-	0/1/1/1	-
9	PEG	N	303	-	-	0/4/4/4	-
7	PG4	L	301	-	-	0/10/10/10	-
7	PG4	M	302	-	-	4/10/10/10	-
9	PEG	O	303	-	-	1/4/4/4	-
5	PGE	B	302	-	-	1/7/7/7	-
6	EDO	H	304	-	-	1/1/1/1	-
9	PEG	K	303	-	-	2/4/4/4	-
5	PGE	P	303	-	-	4/7/7/7	-
6	EDO	G	302	-	-	1/1/1/1	-
5	PGE	M	303	-	-	5/7/7/7	-
9	PEG	E	303	-	-	2/4/4/4	-
5	PGE	C	302	-	-	3/7/7/7	-
6	EDO	J	303	-	-	1/1/1/1	-
9	PEG	F	303	-	-	2/4/4/4	-
8	PG5	L	302	-	-	0/9/9/9	-
6	EDO	C	303	-	-	1/1/1/1	-
6	EDO	M	306	-	-	0/1/1/1	-
6	EDO	D	303	-	-	1/1/1/1	-
6	EDO	D	304	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

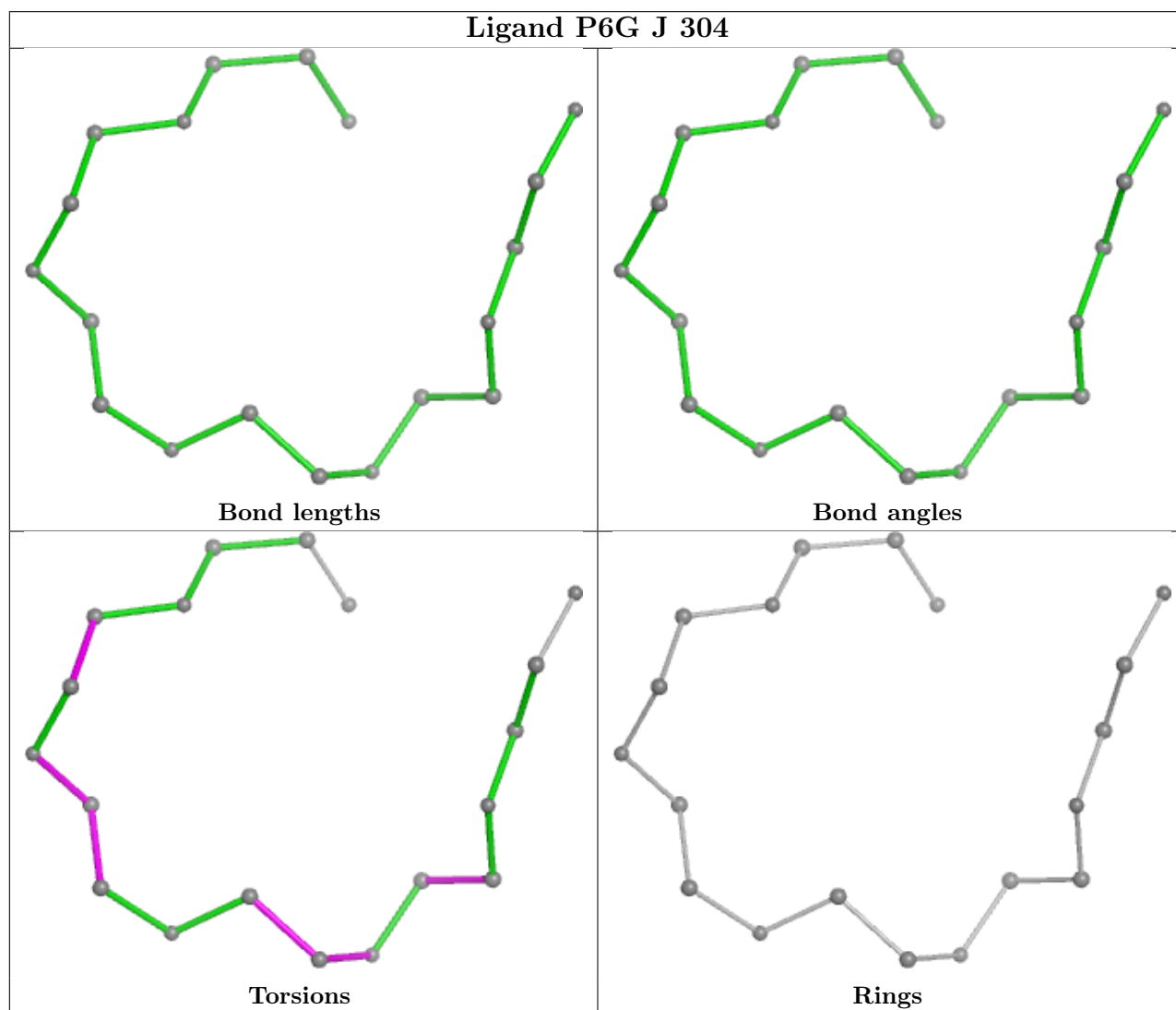
5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	302	PGE	O1-C1-C2-O2
7	N	301	PG4	O2-C3-C4-O3
11	J	304	P6G	O13-C14-C15-O16
11	J	304	P6G	O4-C5-C6-O7
5	P	303	PGE	O2-C3-C4-O3

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 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	218/223 (97%)	0.59	15 (6%)	24 29	16, 45, 71, 100	11 (5%)
1	D	223/223 (100%)	0.92	23 (10%)	13 17	25, 49, 68, 76	19 (8%)
1	G	222/223 (99%)	0.54	14 (6%)	27 33	22, 40, 69, 82	17 (7%)
1	H	215/223 (96%)	0.96	35 (16%)	5 6	27, 49, 81, 121	24 (11%)
1	M	222/223 (99%)	0.39	10 (4%)	39 45	21, 39, 61, 82	11 (4%)
2	B	215/215 (100%)	0.26	5 (2%)	61 67	25, 38, 55, 82	14 (6%)
2	E	212/215 (98%)	1.02	40 (18%)	4 4	29, 50, 87, 111	24 (11%)
2	J	214/215 (99%)	0.29	2 (0%)	81 84	26, 40, 58, 87	9 (4%)
2	L	212/215 (98%)	1.11	45 (21%)	3 3	23, 48, 79, 95	24 (11%)
2	N	214/215 (99%)	0.17	3 (1%)	73 78	26, 38, 51, 67	7 (3%)
3	C	268/300 (89%)	0.13	17 (6%)	27 33	16, 31, 63, 94	13 (4%)
3	F	267/300 (89%)	0.07	14 (5%)	34 40	12, 30, 66, 90	14 (5%)
3	K	273/300 (91%)	-0.05	9 (3%)	49 56	15, 29, 62, 96	8 (2%)
3	O	273/300 (91%)	-0.05	8 (2%)	54 60	15, 29, 60, 95	11 (4%)
3	P	274/300 (91%)	0.14	14 (5%)	34 41	14, 30, 63, 90	17 (6%)
All	All	3522/3690 (95%)	0.40	254 (7%)	23 27	12, 38, 69, 121	223 (6%)

The worst 5 of 254 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	210	PHE	5.3
2	L	193	TYR	5.3
1	H	197	LEU	5.1
1	H	219	VAL	4.8
3	K	20	ILE	4.8

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
5	PGE	M	303	10/10	0.76	0.18	64,66,70,73	0
7	PG4	N	302	13/13	0.80	0.17	60,64,72,73	0
6	EDO	G	302	4/4	0.82	0.15	61,61,62,63	0
9	PEG	D	302	7/7	0.82	0.20	78,79,84,84	0
9	PEG	F	303	7/7	0.82	0.15	72,74,78,78	0
8	PG5	J	301	12/12	0.83	0.15	50,54,58,61	0
7	PG4	B	301	13/13	0.83	0.16	66,67,71,72	0
6	EDO	J	303	4/4	0.83	0.16	59,60,61,63	0
11	P6G	J	304	19/19	0.83	0.18	67,75,79,80	0
7	PG4	N	301	13/13	0.84	0.15	52,56,61,64	0
6	EDO	J	302	4/4	0.84	0.15	65,66,69,69	0
6	EDO	K	305	4/4	0.85	0.17	63,65,66,68	0
6	EDO	D	303	4/4	0.85	0.17	65,65,66,68	0
9	PEG	B	305	7/7	0.86	0.13	62,64,65,66	0
6	EDO	H	305	4/4	0.86	0.15	66,69,70,70	0
6	EDO	C	303	4/4	0.87	0.16	68,69,69,70	0
9	PEG	N	303	7/7	0.87	0.11	74,75,76,77	0
7	PG4	L	301	13/13	0.87	0.17	64,67,71,72	0
5	PGE	C	302	10/10	0.88	0.14	63,66,82,85	0
6	EDO	B	307	4/4	0.88	0.13	66,66,67,69	0
8	PG5	L	302	12/12	0.88	0.14	58,62,64,65	0
5	PGE	H	303	10/10	0.89	0.14	62,64,68,69	0
6	EDO	B	306	4/4	0.89	0.14	63,65,67,68	0
6	EDO	K	304	4/4	0.90	0.10	47,51,51,54	0
6	EDO	F	302	4/4	0.90	0.12	54,54,55,57	0
6	EDO	M	304	4/4	0.90	0.13	52,54,56,57	0
6	EDO	M	306	4/4	0.90	0.14	69,70,70,71	0

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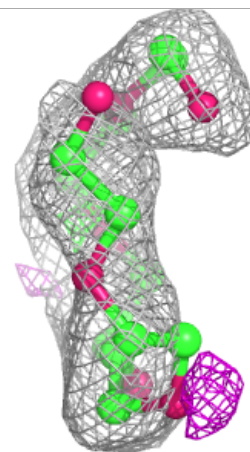
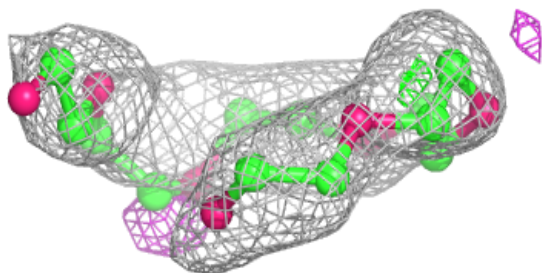
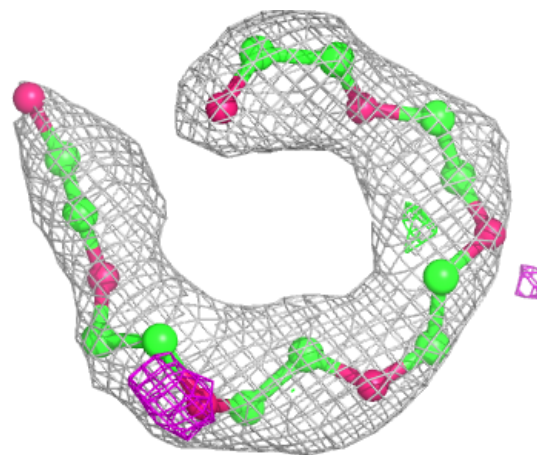
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	D	301	4/4	0.90	0.13	70,70,70,71	0
7	PG4	P	302	13/13	0.90	0.12	47,54,64,65	0
9	PEG	K	303	7/7	0.90	0.15	59,60,62,66	0
5	PGE	E	302	10/10	0.90	0.13	53,57,67,68	0
9	PEG	O	303	7/7	0.90	0.15	65,66,67,71	0
6	EDO	D	304	4/4	0.90	0.13	63,64,66,69	0
6	EDO	K	307	4/4	0.91	0.12	57,58,58,60	0
6	EDO	C	304	4/4	0.91	0.13	54,57,57,62	0
6	EDO	M	305	4/4	0.91	0.10	60,60,62,63	0
7	PG4	M	302	13/13	0.91	0.12	46,50,60,61	0
5	PGE	P	303	10/10	0.91	0.13	59,64,69,70	0
6	EDO	M	307	4/4	0.92	0.10	60,60,61,63	0
5	PGE	B	304	10/10	0.92	0.13	59,60,63,65	0
9	PEG	E	303	7/7	0.92	0.12	60,61,62,63	0
5	PGE	B	303	10/10	0.92	0.10	53,56,62,62	0
6	EDO	P	304	4/4	0.93	0.10	67,69,71,72	0
6	EDO	H	304	4/4	0.93	0.10	54,54,55,57	0
6	EDO	K	306	4/4	0.93	0.14	70,72,72,73	0
5	PGE	H	302	10/10	0.93	0.12	56,57,57,58	0
10	1PE	G	301	16/16	0.93	0.11	43,52,66,67	0
6	EDO	K	308	4/4	0.93	0.12	62,62,63,65	0
9	PEG	O	302	7/7	0.94	0.10	55,57,61,63	0
9	PEG	K	302	7/7	0.94	0.11	54,54,56,56	0
4	CL	A	301	1/1	0.94	0.14	75,75,75,75	0
5	PGE	B	302	10/10	0.94	0.12	51,54,64,64	0
4	CL	M	301	1/1	0.96	0.10	57,57,57,57	0
4	CL	E	301	1/1	0.98	0.11	55,55,55,55	0
4	CL	K	301	1/1	0.98	0.07	35,35,35,35	0
4	CL	H	301	1/1	0.98	0.09	53,53,53,53	0
4	CL	O	301	1/1	0.98	0.05	35,35,35,35	0
4	CL	C	301	1/1	0.98	0.04	35,35,35,35	0
4	CL	P	301	1/1	0.99	0.07	37,37,37,37	0
4	CL	F	301	1/1	0.99	0.04	36,36,36,36	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 P6G J 304:

$2mF_o-DF_c$ (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.