



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:19 PM UTC

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 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

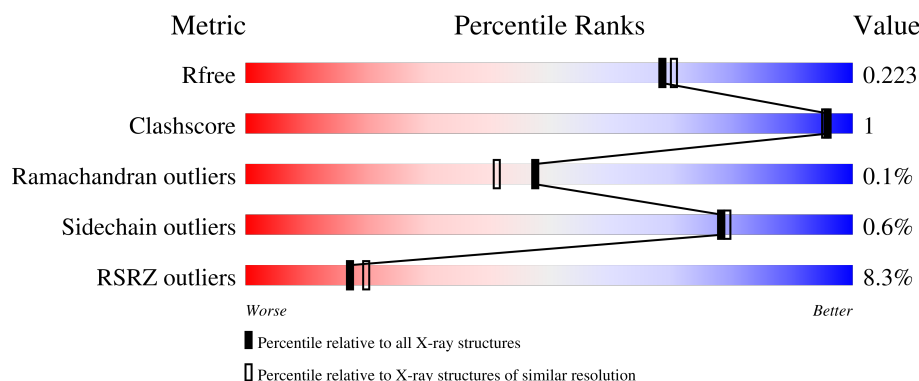
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

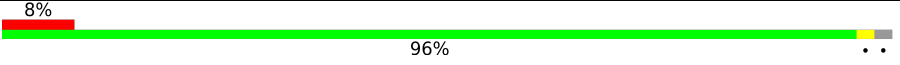
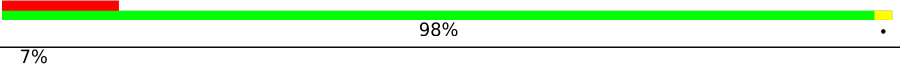
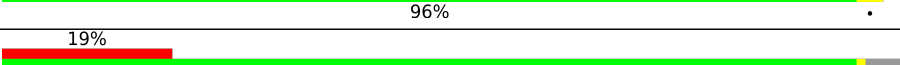
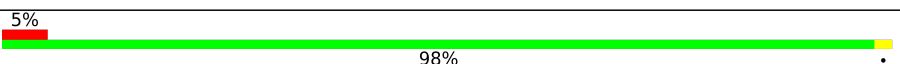
The reported resolution of this entry is 1.96 Å.

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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	
1	D	223	
1	G	223	
1	H	223	
1	M	223	

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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).

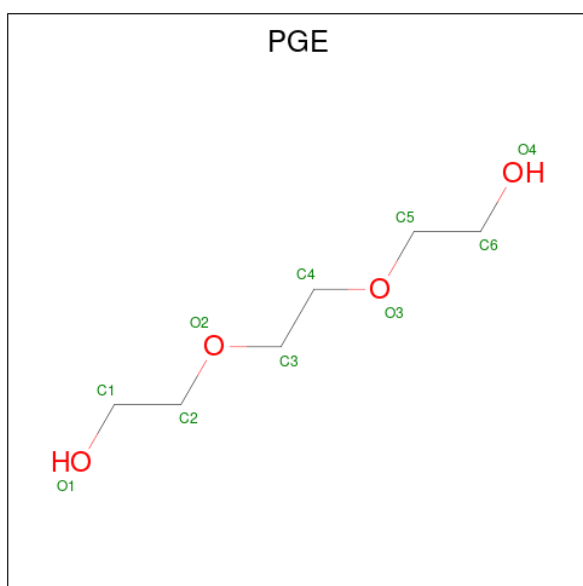
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Cl	0	0
			1	1		
4	P	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

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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: $C_6H_{14}O_4$).



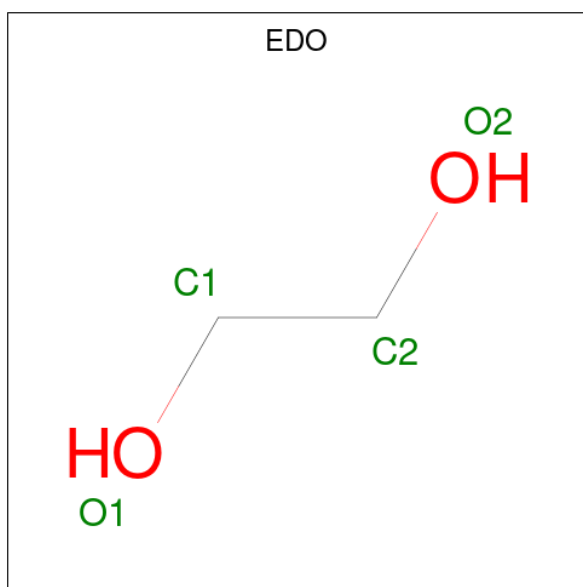
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			10	6	4		
5	H	1	Total	C	O	0	0
			10	6	4		
5	P	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

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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: $C_2H_6O_2$).



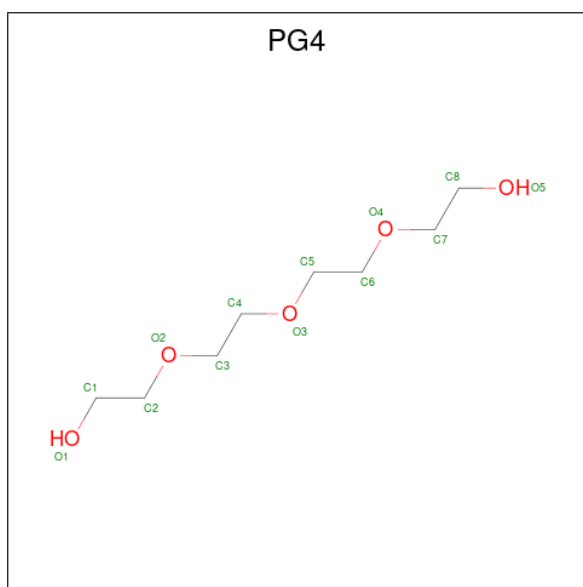
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	P	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

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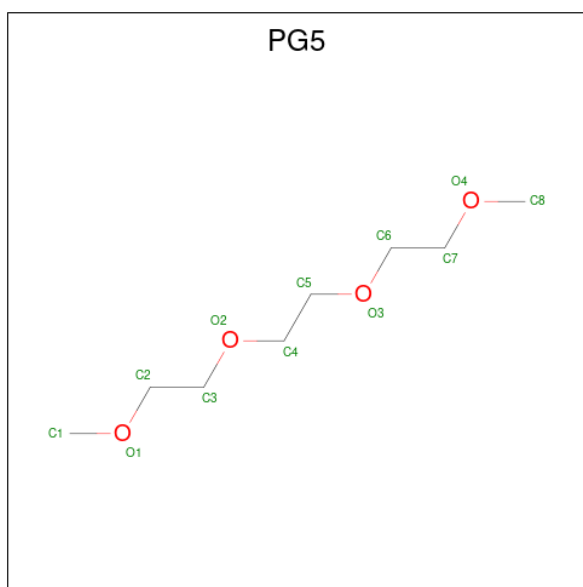
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	K	1	Total	C	O	0	0
			4	2	2		
6	K	1	Total	C	O	0	0
			4	2	2		
6	K	1	Total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

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



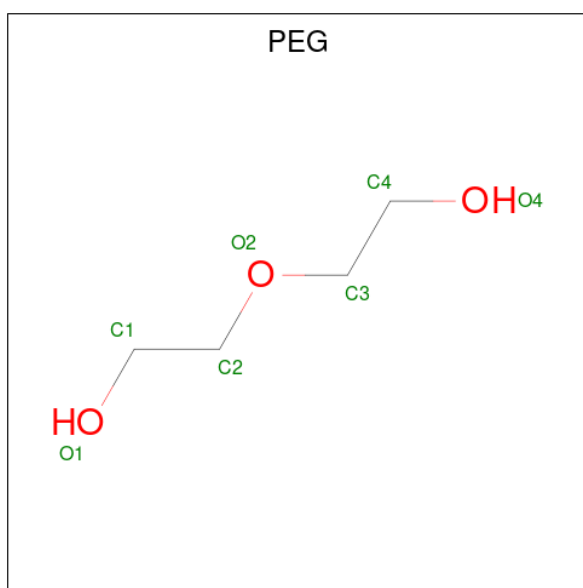
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			13	8	5		
7	P	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	M	1	Total	C	O	0	0
			13	8	5		
7	N	1	Total	C	O	0	0
			13	8	5		
7	N	1	Total	C	O	0	0
			13	8	5		

- 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: $C_4H_{10}O_3$).



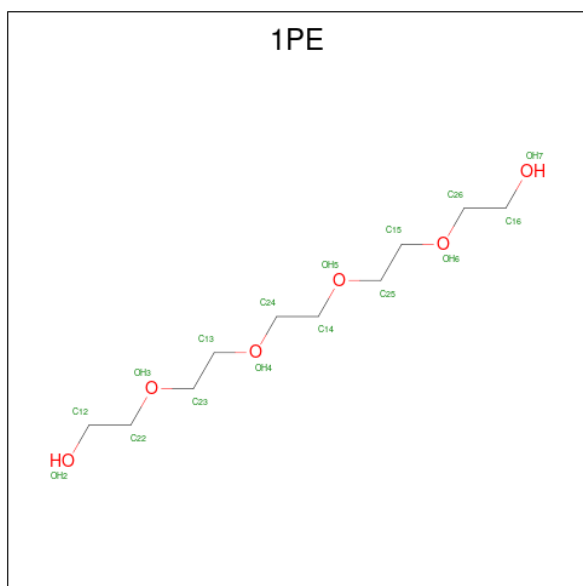
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		

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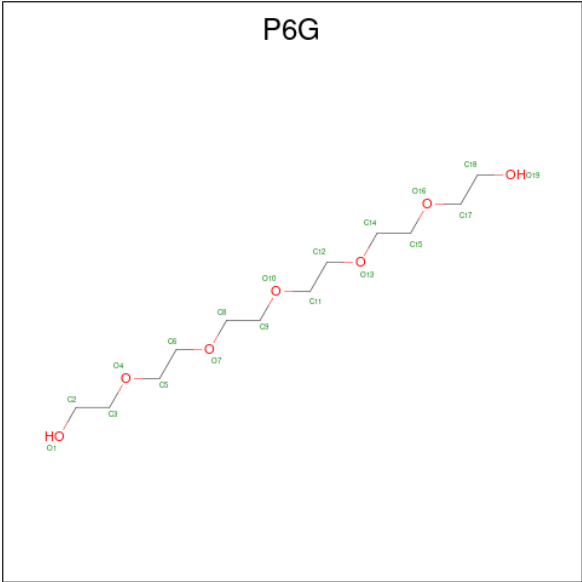
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			7	4	3		
9	F	1	Total	C	O	0	0
			7	4	3		
9	K	1	Total	C	O	0	0
			7	4	3		
9	K	1	Total	C	O	0	0
			7	4	3		
9	N	1	Total	C	O	0	0
			7	4	3		
9	O	1	Total	C	O	0	0
			7	4	3		
9	O	1	Total	C	O	0	0
			7	4	3		

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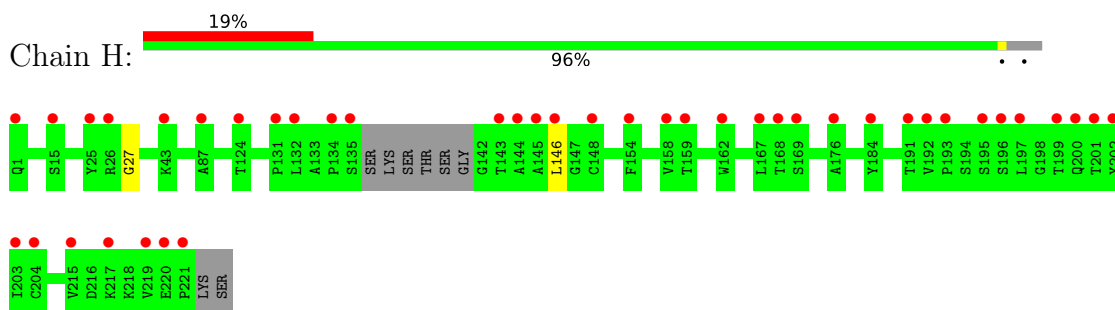
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	K	222	Total 222	O 222	0	0
12	M	124	Total 124	O 124	0	0
12	N	162	Total 162	O 162	0	0
12	O	206	Total 206	O 206	0	0

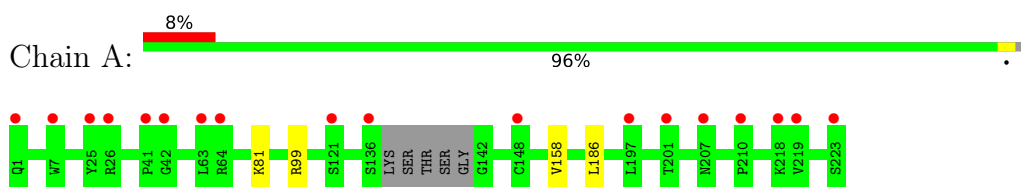
3 Residue-property plots [i](#)

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.

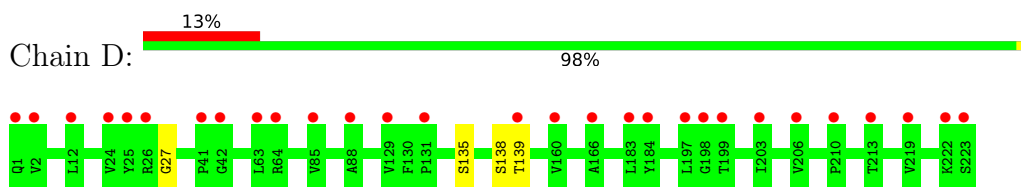
- Molecule 1: 319C07 antibody heavy chain, Fab fragment



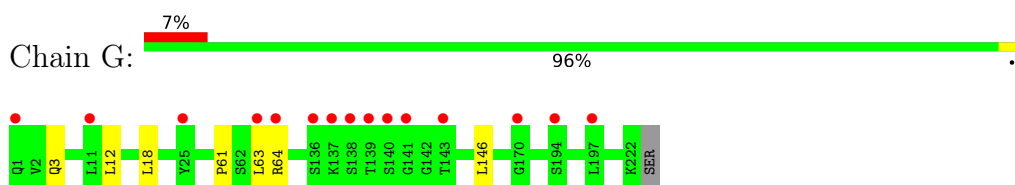
- Molecule 1: 319C07 antibody heavy chain, Fab fragment



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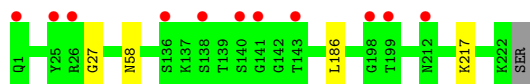


- Molecule 1: 319C07 antibody heavy chain, Fab fragment

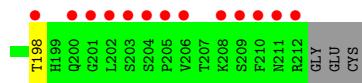
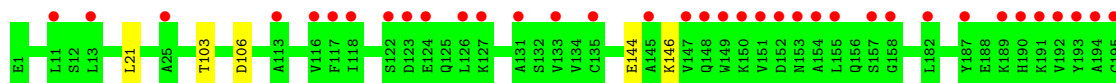


- Molecule 1: 319C07 antibody heavy chain, Fab fragment

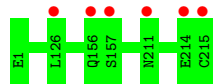




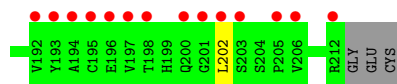
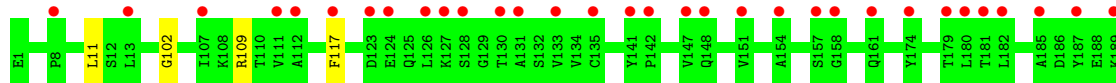
- Molecule 2: 319C07 antibody light chain, Fab fragment



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



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



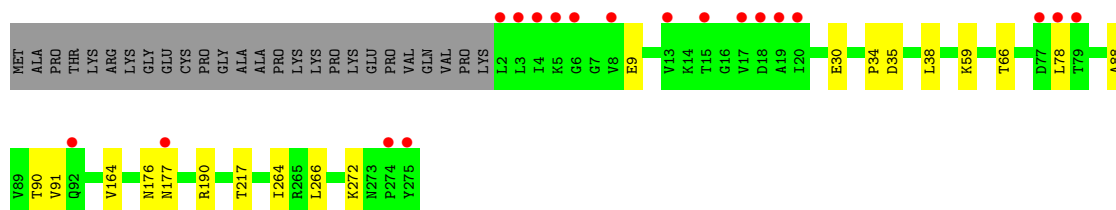
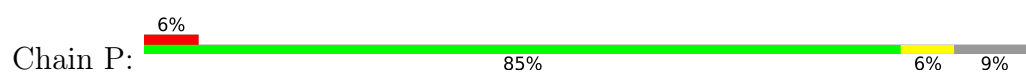
- Molecule 2: 319C07 antibody light chain, Fab fragment



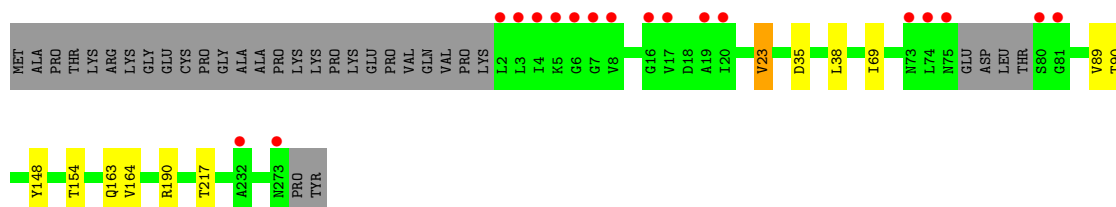
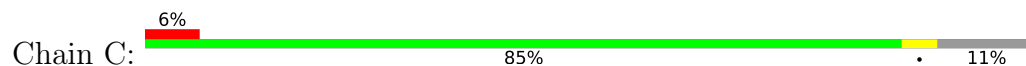
- Molecule 2: 319C07 antibody light chain, Fab fragment



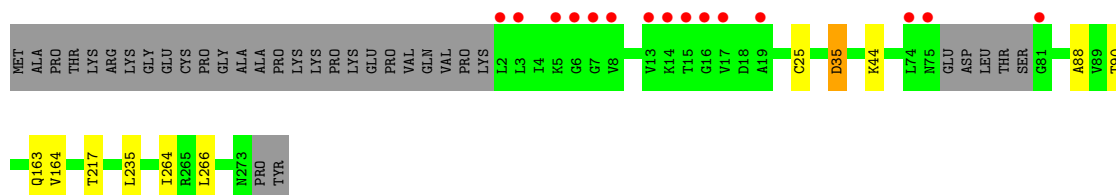
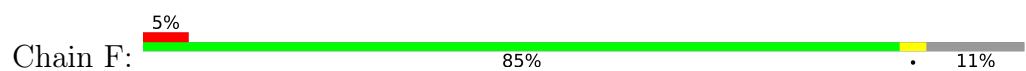
- Molecule 3: Major capsid protein VP1



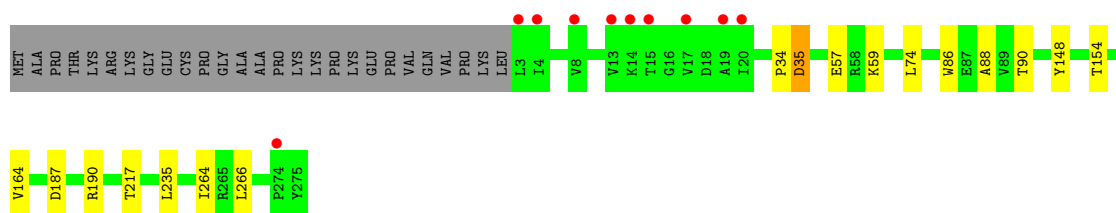
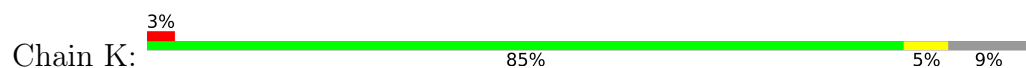
- Molecule 3: Major capsid protein VP1



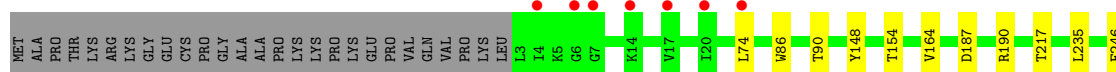
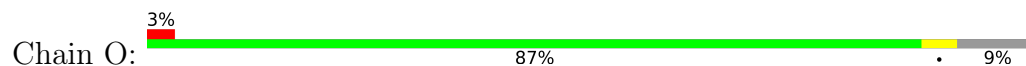
- Molecule 3: Major capsid protein VP1



- 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	13696 reflections (4.61%)	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: PEG, PG5, PGE, 1PE, EDO, CL, P6G, PG4

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.

All (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
2	E	102	GLY	CA-C-O	-5.18	118.66	122.23
2	E	202	LEU	CA-C-N	5.14	127.12	120.44
2	E	202	LEU	C-N-CA	5.14	127.12	120.44
1	H	27	GLY	CA-C-O	-5.00	118.78	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
3:K:235:LEU:HD21	3:K:264:ILE:HD13	1.79	0.63
3:P:190[A]:ARG:HH11	3:P:190[A]:ARG:HG3	1.68	0.58
3:O:235:LEU:HD21	3:O:264:ILE:HD13	1.88	0.56
3:C:23:VAL:CG1	3:C:69:ILE:HG21	2.37	0.54
2:N:162:GLU:HG3	12:N:403:HOH:O	2.07	0.54
3:K:187:ASP:OD2	3:K:190[A]:ARG:HD3	2.10	0.52
3:P:34:PRO:HA	3:P:59:LYS:HD2	1.94	0.49
3:K:190[A]:ARG:NH2	12:K:401:HOH:O	2.40	0.49
3:K:34:PRO:HA	3:K:59:LYS:HD2	1.95	0.49
3:K:74:LEU:HD21	3:K:86:TRP:CZ2	2.48	0.49
3:C:190[B]:ARG:HH11	3:C:190[B]:ARG:HG2	1.73	0.48
3:P:34:PRO:HD2	12:P:452:HOH:O	2.14	0.48
3:C:190[B]:ARG:CG	3:C:190[B]:ARG:NH1	2.56	0.48
3:O:74:LEU:HD21	3:O:86:TRP:CZ2	2.49	0.47
1:G:12:LEU:HD11	1:G:18:LEU:HD13	1.96	0.47
1:D:135:SER:O	1:D:139:THR:HG22	2.15	0.47
3:C:90:THR:HB	3:C:217:THR:CG2	2.46	0.46
3:P:66:THR:O	3:P:176[A]:ASN:ND2	2.42	0.46
3:C:190[B]:ARG:HG2	3:C:190[B]:ARG:NH1	2.31	0.45
3:O:90:THR:HB	3:O:217:THR:CG2	2.47	0.44
2:L:106[B]:ASP:OD1	2:L:106[B]:ASP:C	2.60	0.44
3:P:38:LEU:HA	3:C:163:GLN:HE22	1.81	0.44
12:E:448:HOH:O	3:F:44[B]:LYS:HG2	2.16	0.44
3:C:23:VAL:HG13	3:C:69:ILE:HG21	1.98	0.44
3:P:88:ALA:HA	3:P:266:LEU:HD23	1.99	0.44
3:O:190[B]:ARG:NH2	12:O:403:HOH:O	2.47	0.43
3:P:91:VAL:HG23	3:P:264:ILE:CD1	2.49	0.43
1:G:61:PRO:HA	1:G:64:ARG:HB2	1.99	0.43
1:D:138:SER:HA	2:E:117:PHE:HB3	2.00	0.43
3:P:190[A]:ARG:HH11	3:P:190[A]:ARG:CG	2.29	0.43
3:O:187:ASP:OD2	3:O:190[B]:ARG:HD3	2.18	0.43
3:K:148:TYR:CG	3:K:154:THR:HG21	2.54	0.43
1:A:81:LYS:HG3	12:A:430:HOH:O	2.19	0.42
3:P:90:THR:HB	3:P:217:THR:HG23	2.00	0.42
2:L:146:LYS:HB2	2:L:198:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:90:THR:HB	3:P:217:THR:CG2	2.50	0.42
3:C:148:TYR:CG	3:C:154:THR:HG21	2.55	0.42
3:O:148:TYR:CG	3:O:154:THR:HG21	2.55	0.42
3:F:88:ALA:HA	3:F:266:LEU:HD23	2.01	0.42
2:L:21:LEU:HD22	2:L:103:THR:HG21	2.02	0.41
3:C:38:LEU:HA	3:F:163:GLN:HE22	1.85	0.41
3:C:89:VAL:HG12	3:C:90:THR:HG23	2.02	0.41
3:P:9:GLU:HB3	3:P:272:LYS:HB2	2.03	0.41
3:K:88:ALA:HA	3:K:266:LEU:HD23	2.03	0.41
3:P:30[B]:GLU:OE1	3:P:177:ASN:N	2.52	0.41
1:A:158:VAL:CG1	1:A:186:LEU:HD21	2.49	0.41
3:P:91:VAL:HG23	3:P:264:ILE:HD13	2.03	0.41
3:F:90:THR:HB	3:F:217:THR:CG2	2.50	0.41
3:K:90:THR:HB	3:K:217:THR:CG2	2.51	0.40
1:M:186:LEU:C	1:M:186:LEU:HD12	2.46	0.40
2:N:146:LYS:HB2	2:N:198:THR:OG1	2.20	0.40
3:O:246:PHE:O	3:O:253:GLN:HA	2.22	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	41

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%)	65	64
1	D	192/191 (100%)	192 (100%)	0	100	100
1	G	193/191 (101%)	190 (98%)	3 (2%)	55	52
1	H	184/191 (96%)	183 (100%)	1 (0%)	81	82
1	M	192/191 (100%)	191 (100%)	1 (0%)	81	82
2	B	188/187 (100%)	188 (100%)	0	100	100
2	E	185/187 (99%)	183 (99%)	2 (1%)	65	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	186/187 (100%)	185 (100%)	1 (0%)	81	82
2	L	188/187 (100%)	187 (100%)	1 (0%)	81	82
2	N	186/187 (100%)	186 (100%)	0	100	100
3	C	235/257 (91%)	233 (99%)	2 (1%)	70	70
3	F	233/257 (91%)	232 (100%)	1 (0%)	84	85
3	K	237/257 (92%)	235 (99%)	2 (1%)	73	74
3	O	238/257 (93%)	238 (100%)	0	100	100
3	P	244/257 (95%)	242 (99%)	2 (1%)	73	74
All	All	3069/3175 (97%)	3051 (99%)	18 (1%)	78	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	146	LEU
2	L	144	GLU
3	P	35	ASP
3	P	78	LEU
1	A	99[A]	ARG
1	A	99[B]	ARG
3	C	23	VAL
3	C	35	ASP
2	E	11	LEU
2	E	109	ARG
3	F	35	ASP
1	G	3	GLN
1	G	63	LEU
1	G	146	LEU
2	J	106	ASP
3	K	35	ASP
3	K	57	GLU
1	M	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	52	ASN
2	L	138	ASN

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Mol	Chain	Res	Type
2	L	139	ASN
3	P	92	GLN
3	P	205	ASN
3	P	224	GLN
1	A	3	GLN
1	A	52	ASN
1	A	53	HIS
2	B	138	ASN
2	B	139	ASN
1	D	52	ASN
1	D	172	HIS
2	E	138	ASN
2	E	139	ASN
1	G	53	HIS
2	J	138	ASN
2	J	139	ASN
2	J	161	GLN
3	K	37	ASN
3	K	92	GLN
3	K	161	GLN
1	M	3	GLN
2	N	138	ASN
2	N	139	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
5	PGE	C	302	-	9,9,9	0.17	0	8,8,8	0.14	0
6	EDO	B	307	-	3,3,3	0.15	0	2,2,2	0.36	0
7	PG4	P	302	-	12,12,12	0.17	0	11,11,11	0.17	0
9	PEG	D	302	-	6,6,6	0.18	0	5,5,5	0.16	0
9	PEG	E	303	-	6,6,6	0.14	0	5,5,5	0.11	0
5	PGE	M	303	-	9,9,9	0.21	0	8,8,8	0.18	0
6	EDO	D	304	-	3,3,3	0.09	0	2,2,2	0.23	0
5	PGE	H	302	-	9,9,9	0.13	0	8,8,8	0.16	0
7	PG4	N	301	-	12,12,12	0.19	0	11,11,11	0.25	0
6	EDO	K	304	-	3,3,3	0.12	0	2,2,2	0.30	0
9	PEG	N	303	-	6,6,6	0.14	0	5,5,5	0.10	0
5	PGE	B	303	-	9,9,9	0.21	0	8,8,8	0.18	0
9	PEG	B	305	-	6,6,6	0.17	0	5,5,5	0.10	0
8	PG5	L	302	-	11,11,11	0.18	0	10,10,10	0.18	0
6	EDO	K	306	-	3,3,3	0.10	0	2,2,2	0.22	0
6	EDO	M	306	-	3,3,3	0.11	0	2,2,2	0.22	0
6	EDO	F	302	-	3,3,3	0.16	0	2,2,2	0.41	0
6	EDO	J	303	-	3,3,3	0.17	0	2,2,2	0.24	0
9	PEG	F	303	-	6,6,6	0.23	0	5,5,5	0.19	0
8	PG5	J	301	-	11,11,11	0.21	0	10,10,10	0.24	0
9	PEG	O	302	-	6,6,6	0.16	0	5,5,5	0.17	0
7	PG4	B	301	-	12,12,12	0.22	0	11,11,11	0.16	0
6	EDO	J	302	-	3,3,3	0.09	0	2,2,2	0.21	0
7	PG4	N	302	-	12,12,12	0.21	0	11,11,11	0.22	0
6	EDO	K	308	-	3,3,3	0.12	0	2,2,2	0.37	0
6	EDO	M	304	-	3,3,3	0.13	0	2,2,2	0.25	0
5	PGE	H	303	-	9,9,9	0.20	0	8,8,8	0.16	0
11	P6G	J	304	-	18,18,18	0.23	0	17,17,17	0.27	0
6	EDO	H	304	-	3,3,3	0.14	0	2,2,2	0.34	0
10	1PE	G	301	-	15,15,15	0.21	0	14,14,14	0.24	0
6	EDO	H	305	-	3,3,3	0.10	0	2,2,2	0.20	0
6	EDO	C	304	-	3,3,3	0.16	0	2,2,2	0.37	0
5	PGE	E	302	-	9,9,9	0.17	0	8,8,8	0.15	0
5	PGE	P	303	-	9,9,9	0.23	0	8,8,8	0.17	0
7	PG4	M	302	-	12,12,12	0.17	0	11,11,11	0.21	0
6	EDO	K	305	-	3,3,3	0.14	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PG4	L	301	-	12,12,12	0.19	0	11,11,11	0.16	0
6	EDO	K	307	-	3,3,3	0.08	0	2,2,2	0.26	0
5	PGE	B	302	-	9,9,9	0.16	0	8,8,8	0.19	0
6	EDO	M	307	-	3,3,3	0.07	0	2,2,2	0.20	0
9	PEG	K	303	-	6,6,6	0.16	0	5,5,5	0.11	0
6	EDO	G	302	-	3,3,3	0.12	0	2,2,2	0.25	0
6	EDO	P	304	-	3,3,3	0.16	0	2,2,2	0.38	0
9	PEG	O	303	-	6,6,6	0.17	0	5,5,5	0.13	0
6	EDO	D	303	-	3,3,3	0.08	0	2,2,2	0.23	0
6	EDO	B	306	-	3,3,3	0.13	0	2,2,2	0.29	0
6	EDO	M	305	-	3,3,3	0.08	0	2,2,2	0.23	0
6	EDO	C	303	-	3,3,3	0.11	0	2,2,2	0.30	0
9	PEG	K	302	-	6,6,6	0.18	0	5,5,5	0.20	0
5	PGE	B	304	-	9,9,9	0.17	0	8,8,8	0.20	0
6	EDO	D	301	-	3,3,3	0.06	0	2,2,2	0.22	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
5	PGE	C	302	-	-	3/7/7/7	-
6	EDO	B	307	-	-	1/1/1/1	-
7	PG4	P	302	-	-	2/10/10/10	-
9	PEG	D	302	-	-	2/4/4/4	-
9	PEG	E	303	-	-	2/4/4/4	-
5	PGE	M	303	-	-	5/7/7/7	-
6	EDO	D	304	-	-	0/1/1/1	-
5	PGE	H	302	-	-	3/7/7/7	-
7	PG4	N	301	-	-	7/10/10/10	-
6	EDO	K	304	-	-	1/1/1/1	-
9	PEG	N	303	-	-	0/4/4/4	-
5	PGE	B	303	-	-	3/7/7/7	-
9	PEG	B	305	-	-	1/4/4/4	-
8	PG5	L	302	-	-	0/9/9/9	-
6	EDO	K	306	-	-	1/1/1/1	-
6	EDO	M	306	-	-	0/1/1/1	-
6	EDO	F	302	-	-	1/1/1/1	-
6	EDO	J	303	-	-	1/1/1/1	-
9	PEG	F	303	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PG5	J	301	-	-	2/9/9/9	-
9	PEG	O	302	-	-	3/4/4/4	-
7	PG4	B	301	-	-	2/10/10/10	-
6	EDO	J	302	-	-	0/1/1/1	-
7	PG4	N	302	-	-	5/10/10/10	-
6	EDO	K	308	-	-	1/1/1/1	-
6	EDO	M	304	-	-	0/1/1/1	-
5	PGE	H	303	-	-	4/7/7/7	-
11	P6G	J	304	-	-	6/16/16/16	-
6	EDO	H	304	-	-	1/1/1/1	-
10	1PE	G	301	-	-	3/13/13/13	-
6	EDO	H	305	-	-	1/1/1/1	-
6	EDO	C	304	-	-	1/1/1/1	-
5	PGE	E	302	-	-	3/7/7/7	-
5	PGE	P	303	-	-	4/7/7/7	-
7	PG4	M	302	-	-	4/10/10/10	-
6	EDO	K	305	-	-	1/1/1/1	-
7	PG4	L	301	-	-	0/10/10/10	-
6	EDO	K	307	-	-	1/1/1/1	-
5	PGE	B	302	-	-	1/7/7/7	-
6	EDO	M	307	-	-	0/1/1/1	-
9	PEG	K	303	-	-	2/4/4/4	-
6	EDO	G	302	-	-	1/1/1/1	-
6	EDO	P	304	-	-	1/1/1/1	-
9	PEG	O	303	-	-	1/4/4/4	-
6	EDO	D	303	-	-	1/1/1/1	-
6	EDO	B	306	-	-	1/1/1/1	-
6	EDO	M	305	-	-	0/1/1/1	-
6	EDO	C	303	-	-	1/1/1/1	-
9	PEG	K	302	-	-	3/4/4/4	-
5	PGE	B	304	-	-	1/7/7/7	-
6	EDO	D	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	N	301	PG4	O2-C3-C4-O3
11	J	304	P6G	O13-C14-C15-O16
5	C	302	PGE	O1-C1-C2-O2
11	J	304	P6G	O4-C5-C6-O7
5	P	303	PGE	O2-C3-C4-O3
5	P	303	PGE	O3-C5-C6-O4
5	B	303	PGE	O1-C1-C2-O2
9	F	303	PEG	O2-C3-C4-O4
9	K	302	PEG	O2-C3-C4-O4
9	O	302	PEG	O2-C3-C4-O4
5	H	303	PGE	O3-C5-C6-O4
9	B	305	PEG	O1-C1-C2-O2
11	J	304	P6G	O10-C11-C12-O13
6	H	304	EDO	O1-C1-C2-O2
6	P	304	EDO	O1-C1-C2-O2
6	B	307	EDO	O1-C1-C2-O2
6	C	304	EDO	O1-C1-C2-O2
6	F	302	EDO	O1-C1-C2-O2
6	K	304	EDO	O1-C1-C2-O2
5	P	303	PGE	O1-C1-C2-O2
7	P	302	PG4	O1-C1-C2-O2
9	F	303	PEG	O1-C1-C2-O2
9	O	303	PEG	O1-C1-C2-O2
5	H	302	PGE	O2-C3-C4-O3
5	H	303	PGE	O1-C1-C2-O2
7	N	301	PG4	O4-C7-C8-O5
9	E	303	PEG	O2-C3-C4-O4
9	K	303	PEG	O2-C3-C4-O4
9	D	302	PEG	O2-C3-C4-O4
9	K	303	PEG	O1-C1-C2-O2
6	D	301	EDO	O1-C1-C2-O2
6	G	302	EDO	O1-C1-C2-O2
6	J	303	EDO	O1-C1-C2-O2
6	K	305	EDO	O1-C1-C2-O2
6	K	308	EDO	O1-C1-C2-O2
7	B	301	PG4	O2-C3-C4-O3
7	N	301	PG4	C3-C4-O3-C5
5	M	303	PGE	O2-C3-C4-O3
5	P	303	PGE	C3-C4-O3-C5
7	N	302	PG4	O2-C3-C4-O3
5	C	302	PGE	C1-C2-O2-C3
7	M	302	PG4	O1-C1-C2-O2
9	E	303	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
9	K	302	PEG	C1-C2-O2-C3
5	M	303	PGE	C3-C4-O3-C5
5	E	302	PGE	C6-C5-O3-C4
5	C	302	PGE	O2-C3-C4-O3
7	M	302	PG4	C3-C4-O3-C5
7	N	301	PG4	C5-C6-O4-C7
7	P	302	PG4	O4-C7-C8-O5
9	O	302	PEG	O1-C1-C2-O2
9	O	302	PEG	C1-C2-O2-C3
5	B	303	PGE	C4-C3-O2-C2
7	N	302	PG4	C3-C4-O3-C5
6	H	305	EDO	O1-C1-C2-O2
5	B	302	PGE	C6-C5-O3-C4
5	H	303	PGE	C1-C2-O2-C3
9	D	302	PEG	O1-C1-C2-O2
5	B	304	PGE	C1-C2-O2-C3
5	M	303	PGE	O1-C1-C2-O2
5	M	303	PGE	O3-C5-C6-O4
7	M	302	PG4	O2-C3-C4-O3
6	B	306	EDO	O1-C1-C2-O2
7	N	302	PG4	C6-C5-O3-C4
11	J	304	P6G	C9-C8-O7-C6
5	H	303	PGE	O2-C3-C4-O3
7	N	301	PG4	C8-C7-O4-C6
10	G	301	1PE	C16-C26-OH6-C15
10	G	301	1PE	OH7-C16-C26-OH6
5	H	302	PGE	C3-C4-O3-C5
8	J	301	PG5	C5-C4-O2-C3
7	B	301	PG4	C1-C2-O2-C3
5	M	303	PGE	C4-C3-O2-C2
11	J	304	P6G	O7-C8-C9-O10
6	D	303	EDO	O1-C1-C2-O2
6	K	307	EDO	O1-C1-C2-O2
7	N	302	PG4	C1-C2-O2-C3
8	J	301	PG5	O2-C4-C5-O3
6	C	303	EDO	O1-C1-C2-O2
6	K	306	EDO	O1-C1-C2-O2
5	E	302	PGE	O3-C5-C6-O4
9	K	302	PEG	O1-C1-C2-O2
5	E	302	PGE	C3-C4-O3-C5
5	B	303	PGE	O3-C5-C6-O4
7	N	301	PG4	C6-C5-O3-C4

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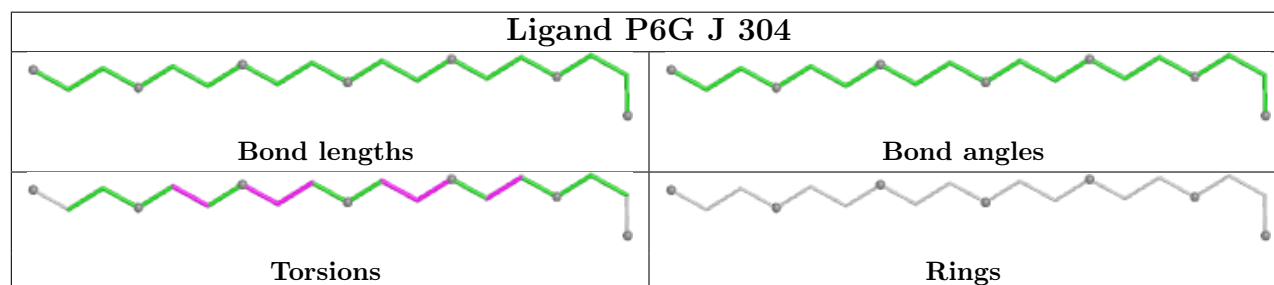
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Mol	Chain	Res	Type	Atoms
5	H	302	PGE	C6-C5-O3-C4
7	M	302	PG4	C1-C2-O2-C3
10	G	301	1PE	C12-C22-OH3-C23
7	N	301	PG4	O3-C5-C6-O4
11	J	304	P6G	C11-C12-O13-C14
7	N	302	PG4	O3-C5-C6-O4

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.70	18 (8%) 17 20	16, 45, 71, 100	11 (5%)
1	D	223/223 (100%)	1.04	29 (13%) 7 8	25, 49, 68, 76	19 (8%)
1	G	222/223 (99%)	0.65	15 (6%) 23 27	22, 40, 69, 82	17 (7%)
1	H	215/223 (96%)	1.08	42 (19%) 3 3	27, 49, 81, 121	24 (11%)
1	M	222/223 (99%)	0.50	11 (4%) 34 40	21, 39, 61, 82	11 (4%)
2	B	215/215 (100%)	0.36	6 (2%) 55 62	25, 38, 55, 82	14 (6%)
2	E	212/215 (98%)	1.14	46 (21%) 2 2	29, 50, 87, 111	24 (11%)
2	J	214/215 (99%)	0.40	2 (0%) 81 85	26, 40, 58, 87	9 (4%)
2	L	212/215 (98%)	1.23	49 (23%) 2 2	23, 48, 79, 95	24 (11%)
2	N	214/215 (99%)	0.27	3 (1%) 73 79	26, 38, 51, 67	7 (3%)
3	C	268/300 (89%)	0.23	18 (6%) 24 27	16, 31, 63, 94	13 (4%)
3	F	267/300 (89%)	0.17	15 (5%) 30 35	12, 30, 66, 90	14 (5%)
3	K	273/300 (91%)	0.06	10 (3%) 45 52	15, 29, 62, 96	8 (2%)
3	O	273/300 (91%)	0.05	8 (2%) 53 60	15, 29, 60, 95	11 (4%)
3	P	274/300 (91%)	0.24	19 (6%) 23 26	14, 30, 63, 90	17 (6%)
All	All	3522/3690 (95%)	0.51	291 (8%) 17 20	12, 38, 69, 121	223 (6%)

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	210	PHE	5.6
2	L	193	TYR	5.5
1	H	197	LEU	5.4
1	H	219	VAL	5.1
3	K	20	ILE	5.0
2	L	206	VAL	4.9
1	G	140	SER	4.8

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Mol	Chain	Res	Type	RSRZ
3	P	15	THR	4.8
2	B	215	CYS	4.7
2	L	205	PRO	4.7
2	L	204	SER	4.6
3	K	4	ILE	4.3
3	C	5	LYS	4.3
1	D	25	TYR	4.2
1	D	198	GLY	4.1
1	G	63	LEU	4.1
1	M	141	GLY	4.0
2	L	192	VAL	4.0
3	C	81	GLY	3.9
1	D	223	SER	3.9
1	H	25	TYR	3.9
1	A	25	TYR	3.9
3	C	4	ILE	3.9
3	C	3	LEU	3.8
3	F	7	GLY	3.8
2	E	212	ARG	3.8
2	L	195	CYS	3.8
1	A	41	PRO	3.8
2	E	201	GLY	3.8
3	F	15	THR	3.7
2	L	191	LYS	3.7
3	O	17	VAL	3.7
3	C	273	ASN	3.7
1	M	25	TYR	3.7
2	L	182	LEU	3.6
2	L	154	ALA	3.6
1	H	1	GLN	3.6
2	L	194	ALA	3.5
3	F	19	ALA	3.5
3	C	6	GLY	3.5
3	C	7	GLY	3.5
1	A	26	ARG	3.5
2	E	157	SER	3.5
1	G	137	LYS	3.5
1	D	63	LEU	3.5
1	G	141	GLY	3.5
1	H	200	GLN	3.5
2	E	123	ASP	3.4
3	P	18	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	L	118	ILE	3.4
2	L	150	LYS	3.4
2	N	204	SER	3.3
3	P	2	LEU	3.3
2	E	205	PRO	3.3
1	M	136	SER	3.3
3	F	2	LEU	3.3
1	G	1	GLN	3.3
2	L	153	ASN	3.3
2	L	157	SER	3.3
3	K	15	THR	3.2
1	H	204	CYS	3.2
2	L	148	GLN	3.2
3	P	4	ILE	3.2
2	E	179	THR	3.2
2	E	206	VAL	3.2
3	P	17	VAL	3.2
2	E	203	SER	3.2
2	L	135	CYS	3.2
2	E	130	THR	3.2
1	H	134	PRO	3.2
2	L	155	LEU	3.2
2	E	196	GLU	3.2
1	H	199	THR	3.1
1	G	139	THR	3.1
1	H	169	SER	3.1
1	A	219	VAL	3.1
2	E	202	LEU	3.1
1	G	64	ARG	3.1
1	A	63	LEU	3.1
1	H	144	ALA	3.1
3	C	74	LEU	3.1
3	K	8	VAL	3.1
2	L	203	SER	3.1
1	D	166	ALA	3.1
3	F	6	GLY	3.1
1	H	195	SER	3.0
2	E	133	VAL	3.0
2	E	192	VAL	3.0
3	C	17	VAL	3.0
1	G	136	SER	3.0
1	H	221	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	131	ALA	3.0
2	L	198	THR	3.0
1	H	145	ALA	3.0
3	K	3	LEU	2.9
3	P	77	ASP	2.9
1	D	203	ILE	2.9
1	D	222	LYS	2.9
1	D	1	GLN	2.9
1	H	203	ILE	2.9
2	B	214	GLU	2.9
2	L	151	VAL	2.9
3	C	16	GLY	2.9
3	C	75	ASN	2.9
3	C	19	ALA	2.9
1	G	197	LEU	2.9
1	H	143	THR	2.8
2	L	211	ASN	2.8
3	K	274	PRO	2.8
1	H	202	TYR	2.8
2	E	174	TYR	2.8
2	L	212	ARG	2.8
2	E	180	LEU	2.8
3	O	20	ILE	2.8
3	K	14	LYS	2.8
2	E	142	PRO	2.8
2	E	151	VAL	2.8
3	C	2	LEU	2.8
1	D	210	PRO	2.8
2	L	133	VAL	2.8
2	L	209	SER	2.7
2	E	185	ALA	2.7
1	M	138	SER	2.7
3	F	5	LYS	2.7
2	L	117	PHE	2.7
1	M	199	THR	2.7
3	P	3	LEU	2.7
1	G	138	SER	2.7
2	L	200	GLN	2.7
1	H	87	ALA	2.7
1	H	196	SER	2.7
2	E	8	PRO	2.7
3	P	20	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	162	TRP	2.6
1	H	217	LYS	2.6
3	C	80	SER	2.6
2	E	147	VAL	2.6
3	F	17	VAL	2.6
1	M	143	THR	2.6
1	G	194	SER	2.6
1	D	183	LEU	2.6
2	E	182	LEU	2.6
3	F	3	LEU	2.6
2	L	152	ASP	2.6
3	F	16	GLY	2.6
1	H	15	SER	2.6
1	H	167	LEU	2.6
2	B	126	LEU	2.6
3	O	6	GLY	2.6
3	O	14	LYS	2.6
2	L	25	ALA	2.6
2	E	194	ALA	2.6
1	A	121	SER	2.6
1	H	148	CYS	2.5
1	H	220	GLU	2.5
1	G	170	GLY	2.5
2	E	197	VAL	2.5
1	M	26	ARG	2.5
2	E	195	CYS	2.5
3	O	275	TYR	2.5
2	L	127	LYS	2.5
1	H	146	LEU	2.5
3	F	81	GLY	2.5
3	O	4	ILE	2.5
1	D	2	VAL	2.5
1	G	143	THR	2.5
2	L	116	VAL	2.5
1	G	25	TYR	2.5
2	L	202	LEU	2.5
3	C	73	ASN	2.5
2	N	7	SER	2.5
1	M	1	GLN	2.5
3	K	19	ALA	2.5
1	A	42	GLY	2.4
2	L	122	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	88	ALA	2.4
1	D	131	PRO	2.4
3	P	177	ASN	2.4
2	L	126	LEU	2.4
2	E	189	LYS	2.4
1	H	201	THR	2.4
3	P	19	ALA	2.4
1	A	64	ARG	2.4
1	H	158	VAL	2.4
1	M	198	GLY	2.4
3	O	7	GLY	2.4
2	L	189	LYS	2.4
3	F	14	LYS	2.4
3	C	20	ILE	2.4
2	N	214	GLU	2.4
1	H	131	PRO	2.4
1	H	193	PRO	2.4
1	D	41	PRO	2.4
1	D	206	VAL	2.4
2	J	158	GLY	2.4
1	H	132	LEU	2.3
2	J	126	LEU	2.3
3	P	275	TYR	2.3
2	E	200	GLN	2.3
2	E	112	ALA	2.3
2	L	147	VAL	2.3
1	A	7	TRP	2.3
1	A	197	LEU	2.3
1	D	139	THR	2.3
2	E	141	TYR	2.3
2	L	145	ALA	2.3
2	E	154	ALA	2.3
2	E	128	SER	2.3
1	D	26	ARG	2.3
1	D	64	ARG	2.3
2	E	135	CYS	2.3
2	L	149	TRP	2.3
3	P	78	LEU	2.3
3	O	74	LEU	2.3
1	A	201	THR	2.3
1	A	218	LYS	2.3
2	L	201	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	158	GLY	2.3
2	L	124	GLU	2.3
2	E	148	GLN	2.3
3	K	13	VAL	2.3
3	F	75	ASN	2.3
2	E	181	THR	2.3
1	H	176	ALA	2.2
1	D	184	TYR	2.2
2	L	113	ALA	2.2
1	M	140	SER	2.2
3	P	13	VAL	2.2
3	C	8	VAL	2.2
2	E	127	LYS	2.2
1	H	26	ARG	2.2
2	E	124	GLU	2.2
2	E	126	LEU	2.2
1	D	42	GLY	2.2
2	L	158	GLY	2.2
1	H	154	PHE	2.2
2	E	193	TYR	2.2
3	F	8	VAL	2.2
1	H	168	THR	2.2
2	B	156	GLN	2.2
3	F	74	LEU	2.2
2	E	117	PHE	2.2
2	L	190	HIS	2.2
1	D	160	VAL	2.2
1	D	213	THR	2.2
2	E	198	THR	2.2
1	H	135	SER	2.2
1	A	148	CYS	2.2
1	D	12	LEU	2.2
3	P	6	GLY	2.2
1	A	210	PRO	2.2
2	E	131	ALA	2.2
2	B	211	ASN	2.1
1	H	124	THR	2.1
1	H	192	VAL	2.1
1	A	136	SER	2.1
1	D	197	LEU	2.1
2	L	11	LEU	2.1
2	L	13	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	13	LEU	2.1
2	L	208	LYS	2.1
3	P	92	GLN	2.1
2	L	123	ASP	2.1
1	D	219	VAL	2.1
3	P	8	VAL	2.1
3	K	17	VAL	2.1
1	A	207	ASN	2.1
2	E	107	ILE	2.1
2	B	157	SER	2.1
1	D	129	VAL	2.1
1	M	212	ASN	2.1
3	F	13	VAL	2.1
3	P	274	PRO	2.1
1	G	11	LEU	2.1
1	A	223	SER	2.0
3	P	5	LYS	2.0
1	H	184	TYR	2.0
2	L	187	TYR	2.0
1	H	159	THR	2.0
3	P	79	THR	2.0
2	E	161	GLN	2.0
1	H	215	VAL	2.0
3	C	232	ALA	2.0
1	H	43	LYS	2.0
1	H	191	THR	2.0
1	A	1	GLN	2.0
1	D	199	THR	2.0
2	E	187	TYR	2.0
1	D	24	VAL	2.0
1	D	85	VAL	2.0
2	E	111	VAL	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
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
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

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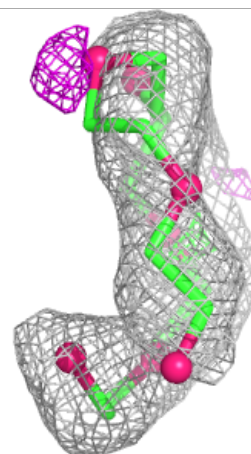
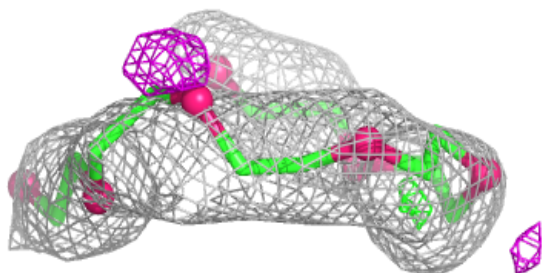
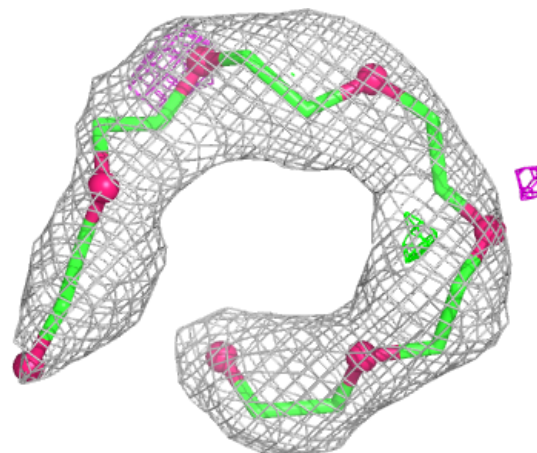
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PGE	P	303	10/10	0.91	0.13	59,64,69,70	0
6	EDO	M	307	4/4	0.92	0.10	60,60,61,63	0
5	PGE	B	304	10/10	0.92	0.13	59,60,63,65	0
9	PEG	E	303	7/7	0.92	0.12	60,61,62,63	0
5	PGE	B	303	10/10	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.