



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:08 AM UTC

PDB ID : 6Z9V / pdb_00006z9v
Title : Human Class I Major Histocompatibility Complex, A02 allele, presenting IIG-WMWIPV
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Deposited on : 2020-06-04
Resolution : 2.01 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

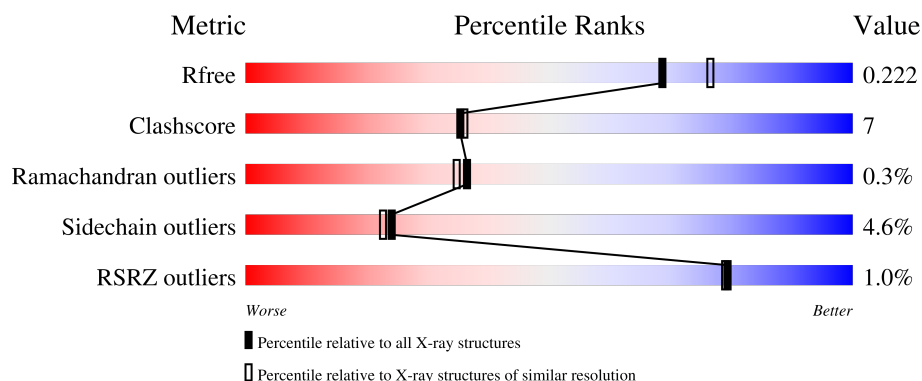
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	276	88% 11% .
1	D	276	84% 15% .
2	B	100	83% 14% ..
2	E	100	83% 15% .
3	C	9	67% 33%

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Mol	Chain	Length	Quality of chain
3	F	9	 67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	D	303	-	-	X	-
5	GOL	D	305	-	-	X	-
5	GOL	D	306	-	-	X	-
9	PE8	D	309	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7063 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	3	0
			2280	1422	416	433	9			
1	D	276	Total	C	N	O	S	0	5	0
			2299	1437	420	433	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			841	537	141	159	4			
2	E	100	Total	C	N	O	S	0	2	0
			849	541	142	162	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called ILE-ILE-GLY-TRP-MET-TRP-ILE-PRO-VAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			79	57	11	10	1			
3	F	9	Total	C	N	O	S	0	0	0
			79	57	11	10	1			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

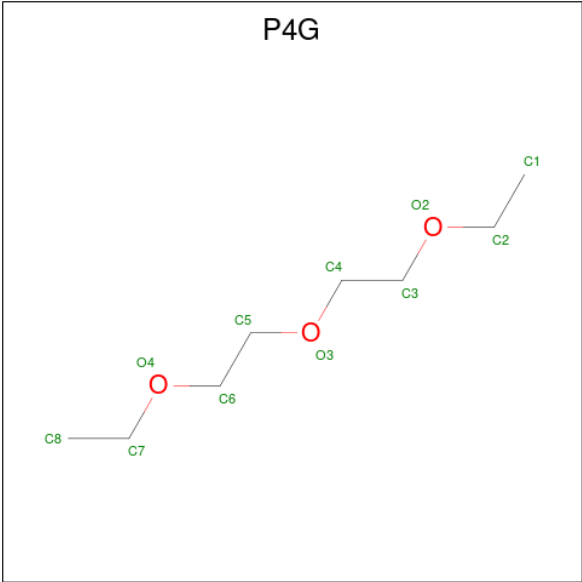


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

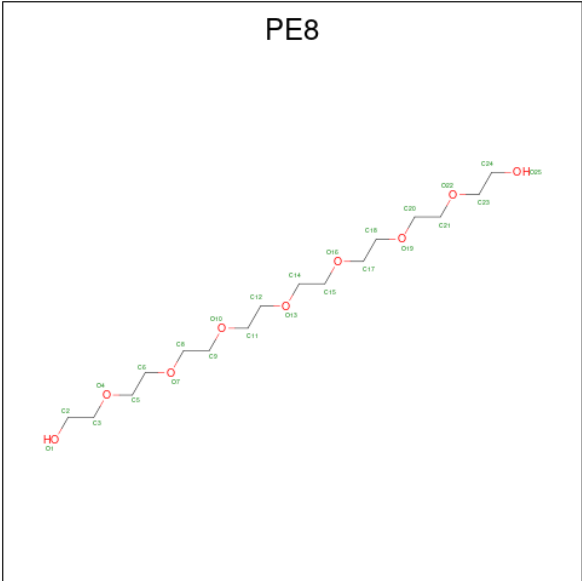
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		

- Molecule 8 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (CCD ID: P4G) (formula: C₈H₁₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			11	8	3		
8	D	1	Total	C	O	0	0
			11	8	3		

- Molecule 9 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: C₁₆H₃₄O₉).



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

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	E	1	Total 1	Ca 1	0	0

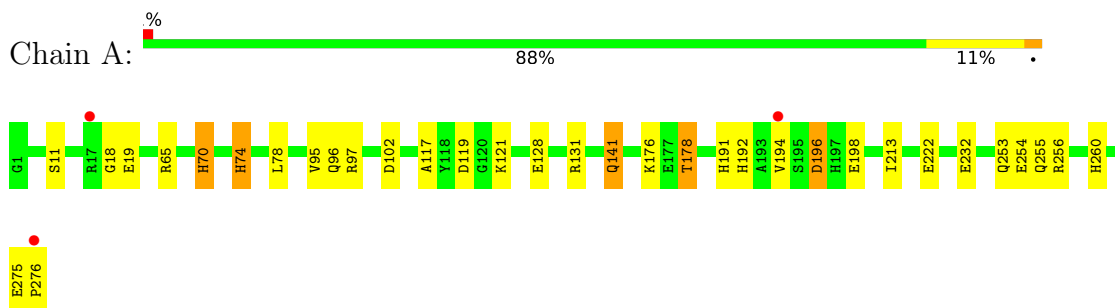
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	171	Total 171	O 171	0	0
11	B	73	Total 73	O 73	0	0
11	C	2	Total 2	O 2	0	0
11	D	163	Total 163	O 163	0	0
11	E	80	Total 80	O 80	0	0
11	F	2	Total 2	O 2	0	0

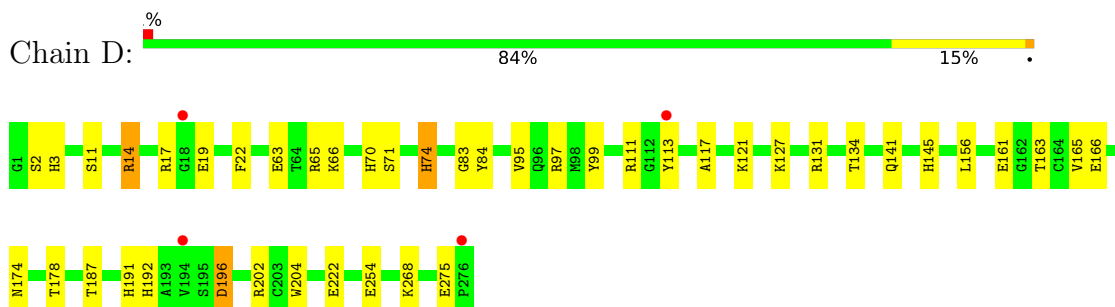
3 Residue-property plots

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.

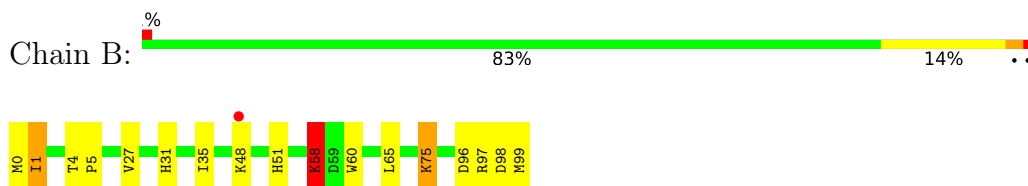
- Molecule 1: MHC class I antigen



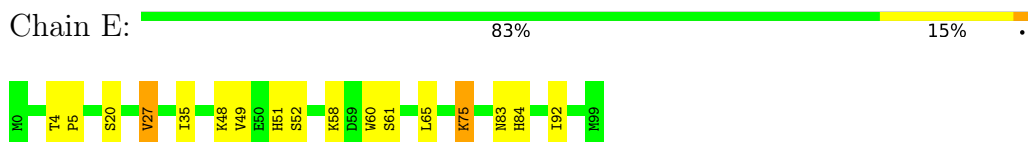
- Molecule 1: MHC class I antigen



- Molecule 2: Beta-2-microglobulin

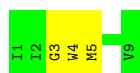


- Molecule 2: Beta-2-microglobulin



- Molecule 3: ILE-ILE-GLY-TRP-MET-TRP-ILE-PRO-VAL

Chain C:  67% 33%



● Molecule 3: ILE-ILE-GLY-TRP-MET-TRP-ILE-PRO-VAL

Chain F:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	85.19Å 85.19Å 232.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	73.78 – 2.01 73.78 – 2.01	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.78-2.01) 100.0 (73.78-2.01)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.02Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.216 0.185 , 0.222	Depositor DCC
R_{free} test set	3287 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7063	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: EDO, P4G, NA, GOL, SO4, PE8, CA

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	1.13	3/2346 (0.1%)	1.34	7/3183 (0.2%)
1	D	1.17	2/2367 (0.1%)	1.34	2/3212 (0.1%)
2	B	1.15	2/867 (0.2%)	1.25	1/1172 (0.1%)
2	E	1.16	3/875 (0.3%)	1.26	1/1183 (0.1%)
3	C	1.11	0/83	1.10	0/113
3	F	1.16	0/83	1.19	0/113
All	All	1.15	10/6621 (0.2%)	1.31	11/8976 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	92	ILE	C-O	-6.12	1.17	1.24
2	E	61	SER	C-O	6.03	1.31	1.23
2	E	49	VAL	C-O	-5.87	1.17	1.24
1	A	260	HIS	CE1-NE2	5.86	1.38	1.32
2	B	5	PRO	C-O	-5.78	1.17	1.23
2	B	58	LYS	C-O	-5.66	1.17	1.24
1	A	70	HIS	CE1-NE2	5.38	1.38	1.32
1	D	145	HIS	CE1-NE2	5.21	1.37	1.32
1	A	198	GLU	CD-OE2	5.13	1.35	1.25
1	D	3	HIS	CE1-NE2	5.12	1.37	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	CG-CD-NE	-6.60	97.47	112.00
1	A	232	GLU	CB-CA-C	6.28	120.14	109.72
1	A	78	LEU	CA-C-N	6.17	126.79	119.94
1	A	78	LEU	C-N-CA	6.17	126.79	119.94
1	A	70	HIS	CA-CB-CG	-5.65	108.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	SER	CA-C-O	-5.53	115.28	121.81
2	B	4	THR	CB-CA-C	5.26	116.43	108.86
1	A	102	ASP	CA-CB-CG	5.13	117.73	112.60
2	E	4	THR	CB-CA-C	5.11	116.08	108.87
1	A	213	ILE	CA-C-O	-5.03	116.74	120.96
1	D	178	THR	CA-CB-OG1	-5.02	102.07	109.60

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	2280	0	2124	19	0
1	D	2299	0	2141	47	0
2	B	841	0	812	16	0
2	E	849	0	815	9	0
3	C	79	0	83	4	0
3	F	79	0	83	4	0
4	A	8	0	12	0	0
4	B	8	0	12	0	0
4	C	4	0	6	0	0
4	D	8	0	12	0	0
4	E	12	0	18	0	0
5	A	6	0	8	1	0
5	D	24	0	32	19	0
5	E	6	0	8	0	0
6	A	15	0	0	0	0
6	D	5	0	0	0	0
7	B	1	0	0	0	0
8	C	11	0	18	4	0
8	D	11	0	18	3	0
9	D	25	0	34	9	0
10	E	1	0	0	0	0
11	A	171	0	0	5	0
11	B	73	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	2	0	0	0	0
11	D	163	0	0	2	0
11	E	80	0	0	0	0
11	F	2	0	0	0	0
All	All	7063	0	6236	95	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 7.

All (95) 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:70:HIS:HE1	1:A:97:ARG:HE	1.24	0.84
1:D:84:TYR:CD1	5:D:305:GOL:H31	2.14	0.82
1:D:65:ARG:HD2	8:D:308:P4G:H12	1.68	0.76
9:D:309:PE8:H211	3:F:4:TRP:HZ2	1.48	0.76
2:B:1:ILE:C	2:B:1:ILE:HD12	2.13	0.74
1:A:70:HIS:HE1	1:A:97:ARG:NE	1.88	0.71
9:D:309:PE8:H211	3:F:4:TRP:CZ2	2.25	0.70
1:D:111:ARG:HD3	11:D:552:HOH:O	1.91	0.70
1:A:70:HIS:CE1	1:A:97:ARG:HE	2.08	0.70
2:B:31:HIS:HD2	11:B:257:HOH:O	1.76	0.68
1:A:141:GLN:CD	11:A:461:HOH:O	2.37	0.67
1:D:192:HIS:HB2	5:D:306:GOL:C1	2.26	0.66
1:D:166:GLU:HG2	9:D:309:PE8:H92	1.78	0.65
1:D:83:GLY:C	5:D:305:GOL:H32	2.22	0.64
2:E:75:LYS:H	2:E:75:LYS:HD2	1.64	0.63
1:D:83:GLY:HA3	5:D:305:GOL:H32	1.80	0.62
1:A:178:THR:HG23	11:A:561:HOH:O	2.00	0.61
1:D:84:TYR:HD1	5:D:305:GOL:H31	1.64	0.60
1:D:174:ASN:ND2	11:D:402:HOH:O	2.33	0.60
2:E:83:ASN:HD22	2:E:84:HIS:H	1.49	0.60
1:D:66:LYS:O	1:D:70[A]:HIS:HD2	1.85	0.59
1:D:111:ARG:HD2	1:D:113:TYR:OH	2.02	0.59
1:A:141:GLN:CG	11:A:461:HOH:O	2.52	0.58
1:A:253:GLN:NE2	1:A:256:ARG:HH11	2.02	0.57
2:B:27[B]:VAL:HG11	2:B:35:ILE:CD1	2.34	0.57
2:E:75:LYS:H	2:E:75:LYS:CD	2.18	0.56
1:A:141:GLN:HG2	11:A:461:HOH:O	2.05	0.56
1:D:83:GLY:CA	5:D:305:GOL:H32	2.36	0.56
1:D:192:HIS:HB2	5:D:306:GOL:C3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:HIS:HB2	5:D:306:GOL:C2	2.37	0.55
1:D:70[B]:HIS:CE1	1:D:97:ARG:HE	2.25	0.55
2:B:27[B]:VAL:HG11	2:B:35:ILE:HD11	1.89	0.54
1:D:70[A]:HIS:HE1	1:D:99:TYR:OH	1.91	0.54
2:B:58:LYS:HA	2:B:58:LYS:HE3	1.88	0.54
1:D:70[B]:HIS:HE1	1:D:97:ARG:NE	2.05	0.54
3:C:5:MET:H	8:C:102:P4G:C3	2.21	0.53
1:D:166:GLU:CG	9:D:309:PE8:H92	2.38	0.53
2:B:1:ILE:HD12	2:B:1:ILE:O	2.08	0.53
1:A:11[B]:SER:OG	1:A:74:HIS:HD2	1.90	0.53
9:D:309:PE8:H172	3:F:1:ILE:HD11	1.89	0.53
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.53
1:D:99:TYR:CD2	5:D:303:GOL:H31	2.44	0.53
1:D:192:HIS:HB2	5:D:306:GOL:H11	1.89	0.53
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.45	0.52
1:D:22[A]:PHE:CG	1:D:71:SER:HB3	2.44	0.51
1:A:178:THR:CG2	11:A:561:HOH:O	2.57	0.51
1:D:84:TYR:CD1	5:D:305:GOL:H11	2.45	0.51
1:D:99:TYR:CE1	5:D:303:GOL:H32	2.46	0.50
2:B:31:HIS:CD2	11:B:257:HOH:O	2.59	0.50
1:D:163:THR:HG23	9:D:309:PE8:H151	1.94	0.50
1:D:202:ARG:NH1	5:D:306:GOL:H2	2.28	0.49
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.95	0.49
1:D:70[A]:HIS:CD2	3:F:6:TRP:HE1	2.31	0.48
2:E:27[B]:VAL:HG11	2:E:35:ILE:CD1	2.42	0.48
1:D:11[A]:SER:HB3	1:D:95:VAL:CG2	2.43	0.48
1:D:84:TYR:HD1	5:D:305:GOL:H11	1.78	0.48
1:D:192:HIS:HB2	5:D:306:GOL:H31	1.94	0.48
1:D:70[B]:HIS:CE1	1:D:97:ARG:NE	2.82	0.47
1:D:11[A]:SER:HB3	1:D:95:VAL:HG22	1.96	0.47
3:C:5:MET:H	8:C:102:P4G:H32	1.79	0.47
1:D:99:TYR:CE2	5:D:303:GOL:H31	2.51	0.46
1:D:63:GLU:OE2	9:D:309:PE8:H241	2.16	0.46
1:A:11[B]:SER:HB2	1:A:95:VAL:CG2	2.46	0.45
1:D:70[B]:HIS:NE2	1:D:74:HIS:CE1	2.85	0.45
1:D:14:ARG:HD3	1:D:19:GLU:O	2.17	0.45
1:D:70[A]:HIS:CE1	1:D:99:TYR:OH	2.70	0.45
8:D:308:P4G:C3	9:D:309:PE8:H212	2.47	0.44
2:E:27[B]:VAL:HG11	2:E:35:ILE:HD11	1.98	0.44
1:A:119:ASP:HB3	2:B:0:MET:HA	1.99	0.44
1:D:192:HIS:CB	5:D:306:GOL:C1	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:HIS:HE1	1:A:254:GLU:OE1	2.01	0.43
2:B:75:LYS:HG3	11:B:224:HOH:O	2.17	0.43
3:C:3:GLY:HA2	8:C:102:P4G:H61	2.00	0.43
1:D:187:THR:HA	1:D:204:TRP:O	2.18	0.43
2:B:51:HIS:HA	2:B:65:LEU:O	2.18	0.43
1:D:196:ASP:OD1	1:D:196:ASP:N	2.50	0.42
2:E:51:HIS:HA	2:E:65:LEU:O	2.19	0.42
1:D:161:GLU:O	9:D:309:PE8:O4	2.36	0.42
1:A:11[A]:SER:HB3	1:A:95:VAL:CG2	2.48	0.42
1:A:192:HIS:HB2	5:A:303:GOL:C3	2.49	0.42
1:D:127:LYS:HE2	1:D:134:THR:OG1	2.20	0.42
1:D:65:ARG:NH2	8:D:308:P4G:O2	2.53	0.42
1:D:192:HIS:N	5:D:306:GOL:H11	2.35	0.42
2:B:97:ARG:HB2	11:B:233:HOH:O	2.20	0.41
2:E:5:PRO:HB2	2:E:27[B]:VAL:HG13	2.02	0.41
3:C:4:TRP:N	8:C:102:P4G:H32	2.35	0.41
2:B:98:ASP:C	2:B:99:MET:HG2	2.45	0.41
2:E:51:HIS:HD2	2:E:52:SER:O	2.03	0.41
1:A:255:GLN:HE22	1:A:276:PRO:HD3	1.86	0.41
1:D:11[B]:SER:OG	1:D:74:HIS:HD2	2.04	0.41
1:A:196:ASP:OD1	1:A:196:ASP:N	2.53	0.41
1:D:156:LEU:CD2	5:D:303:GOL:H2	2.51	0.41
2:B:27[B]:VAL:HG11	2:B:35:ILE:HD13	2.03	0.40
2:B:96:ASP:HB3	2:B:99:MET:HG3	2.04	0.40
1:D:191:HIS:HE1	1:D:254:GLU:OE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	277/276 (100%)	274 (99%)	2 (1%)	1 (0%)	30 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	279/276 (101%)	274 (98%)	4 (1%)	1 (0%)	30	27
2	B	99/100 (99%)	97 (98%)	2 (2%)	0	100	100
2	E	100/100 (100%)	98 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	769/770 (100%)	755 (98%)	12 (2%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	17	ARG
1	A	18	GLY

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	235/232 (101%)	223 (95%)	12 (5%)	21	19
1	D	237/232 (102%)	226 (95%)	11 (5%)	24	22
2	B	96/95 (101%)	92 (96%)	4 (4%)	26	25
2	E	97/95 (102%)	91 (94%)	6 (6%)	16	13
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	8 (100%)	0	100	100
All	All	681/670 (102%)	648 (95%)	33 (5%)	24	21

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	74	HIS
1	A	121	LYS
1	A	128	GLU

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Mol	Chain	Res	Type
1	A	131	ARG
1	A	141	GLN
1	A	176	LYS
1	A	178	THR
1	A	194	VAL
1	A	196	ASP
1	A	222	GLU
1	A	275	GLU
2	B	1	ILE
2	B	48	LYS
2	B	58	LYS
2	B	75	LYS
1	D	14	ARG
1	D	74	HIS
1	D	121	LYS
1	D	131	ARG
1	D	141	GLN
1	D	165[A]	VAL
1	D	165[B]	VAL
1	D	196	ASP
1	D	222	GLU
1	D	268	LYS
1	D	275	GLU
2	E	20	SER
2	E	27[A]	VAL
2	E	27[B]	VAL
2	E	48	LYS
2	E	58	LYS
2	E	75	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	70	HIS
1	A	74	HIS
1	A	155	GLN
1	A	174	ASN
1	A	191	HIS
1	A	226	GLN
1	A	253	GLN
1	A	255	GLN

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Mol	Chain	Res	Type
2	B	31	HIS
2	B	51	HIS
1	D	54	GLN
1	D	72	GLN
1	D	74	HIS
1	D	141	GLN
1	D	174	ASN
1	D	191	HIS
2	E	13	HIS
2	E	51	HIS
2	E	83	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 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	$\# Z > 2$
4	EDO	E	302	-	3,3,3	0.07	0	2,2,2	0.20	0
5	GOL	A	303	-	5,5,5	0.08	0	5,5,5	0.43	0
4	EDO	A	301	-	3,3,3	0.30	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	302	-	3,3,3	0.19	0	2,2,2	0.21	0
6	SO4	D	307	-	4,4,4	0.32	0	6,6,6	0.12	0
5	GOL	D	305	-	5,5,5	0.31	0	5,5,5	1.03	0
4	EDO	C	101	-	3,3,3	0.14	0	2,2,2	0.15	0
6	SO4	A	305	-	4,4,4	0.29	0	6,6,6	0.10	0
4	EDO	E	303	-	3,3,3	0.35	0	2,2,2	0.60	0
4	EDO	E	304	-	3,3,3	0.20	0	2,2,2	0.19	0
5	GOL	D	306	-	5,5,5	0.16	0	5,5,5	0.48	0
5	GOL	D	304	-	5,5,5	0.13	0	5,5,5	0.40	0
5	GOL	E	305	-	5,5,5	0.18	0	5,5,5	0.58	0
4	EDO	A	302	-	3,3,3	0.05	0	2,2,2	0.10	0
5	GOL	D	303	-	5,5,5	0.18	0	5,5,5	0.63	0
4	EDO	D	301	-	3,3,3	0.27	0	2,2,2	0.22	0
4	EDO	B	103	-	3,3,3	0.28	0	2,2,2	0.11	0
6	SO4	A	304	-	4,4,4	0.29	0	6,6,6	0.10	0
8	P4G	C	102	-	10,10,10	0.70	0	9,9,9	0.73	0
8	P4G	D	308	-	10,10,10	0.80	0	9,9,9	0.72	0
4	EDO	B	102	-	3,3,3	0.66	0	2,2,2	0.77	0
6	SO4	A	306	-	4,4,4	0.34	0	6,6,6	0.05	0
9	PE8	D	309	-	24,24,24	0.36	0	23,23,23	0.31	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	EDO	E	302	-	-	1/1/1/1	-
5	GOL	A	303	-	-	2/4/4/4	-
4	EDO	A	301	-	-	1/1/1/1	-
4	EDO	D	302	-	-	1/1/1/1	-
5	GOL	D	305	-	-	4/4/4/4	-
4	EDO	C	101	-	-	0/1/1/1	-
4	EDO	E	303	-	-	0/1/1/1	-
4	EDO	E	304	-	-	1/1/1/1	-
5	GOL	D	306	-	-	4/4/4/4	-
5	GOL	D	304	-	-	2/4/4/4	-
5	GOL	E	305	-	-	2/4/4/4	-
4	EDO	A	302	-	-	0/1/1/1	-
5	GOL	D	303	-	-	2/4/4/4	-
4	EDO	D	301	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	103	-	-	1/1/1/1	-
8	P4G	C	102	-	-	4/8/8/8	-
8	P4G	D	308	-	-	2/8/8/8	-
4	EDO	B	102	-	-	0/1/1/1	-
9	PE8	D	309	-	-	7/22/22/22	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	303	GOL	C1-C2-C3-O3
5	D	304	GOL	C1-C2-C3-O3
5	D	305	GOL	O1-C1-C2-C3
5	D	305	GOL	C1-C2-C3-O3
5	D	306	GOL	O1-C1-C2-C3
5	E	305	GOL	C1-C2-C3-O3
9	D	309	PE8	O7-C8-C9-O10
8	D	308	P4G	O2-C3-C4-O3
8	C	102	P4G	O2-C3-C4-O3
5	D	303	GOL	O1-C1-C2-O2
8	C	102	P4G	O3-C5-C6-O4
5	D	303	GOL	O1-C1-C2-C3
5	D	306	GOL	C1-C2-C3-O3
5	D	305	GOL	O1-C1-C2-O2
5	D	305	GOL	O2-C2-C3-O3
5	D	306	GOL	O1-C1-C2-O2
5	E	305	GOL	O2-C2-C3-O3
4	E	302	EDO	O1-C1-C2-O2
5	A	303	GOL	O2-C2-C3-O3
9	D	309	PE8	O16-C17-C18-O19
5	D	304	GOL	O2-C2-C3-O3
9	D	309	PE8	O10-C11-C12-O13
9	D	309	PE8	C6-C5-O4-C3
4	D	302	EDO	O1-C1-C2-O2
5	D	306	GOL	O2-C2-C3-O3
8	C	102	P4G	C1-C2-O2-C3
8	D	308	P4G	C8-C7-O4-C6
4	B	103	EDO	O1-C1-C2-O2

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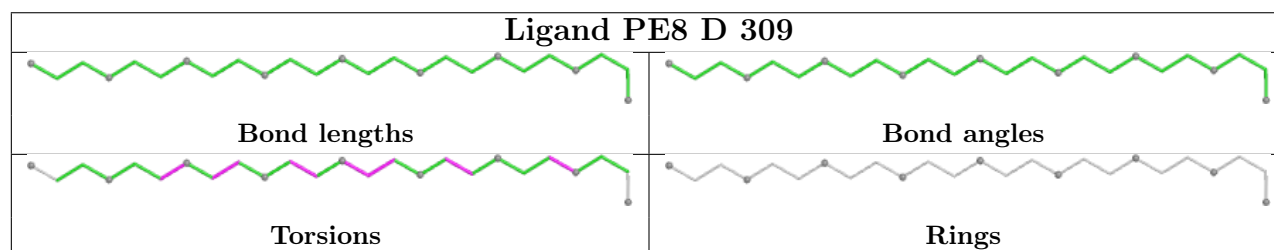
Mol	Chain	Res	Type	Atoms
4	E	304	EDO	O1-C1-C2-O2
9	D	309	PE8	C11-C12-O13-C14
9	D	309	PE8	O13-C14-C15-O16
9	D	309	PE8	C21-C20-O19-C18
8	C	102	P4G	C6-C5-O3-C4
4	A	301	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	303	GOL	1	0
5	D	305	GOL	7	0
5	D	306	GOL	8	0
5	D	303	GOL	4	0
8	C	102	P4G	4	0
8	D	308	P4G	3	0
9	D	309	PE8	9	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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	-0.06	3 (1%) 78 77	13, 34, 57, 88	3 (1%)
1	D	276/276 (100%)	-0.03	4 (1%) 73 73	13, 35, 61, 87	5 (1%)
2	B	100/100 (100%)	0.02	1 (1%) 79 79	15, 36, 57, 72	1 (1%)
2	E	100/100 (100%)	-0.09	0 100 100	17, 37, 56, 63	2 (2%)
3	C	9/9 (100%)	-0.32	0 100 100	29, 30, 33, 42	0
3	F	9/9 (100%)	-0.01	0 100 100	28, 32, 41, 46	0
All	All	770/770 (100%)	-0.05	8 (1%) 79 79	13, 35, 58, 88	11 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	PRO	3.2
2	B	48	LYS	2.7
1	D	18	GLY	2.5
1	A	17	ARG	2.5
1	D	194	VAL	2.4
1	A	194	VAL	2.3
1	D	113	TYR	2.2
1	D	276	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

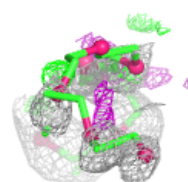
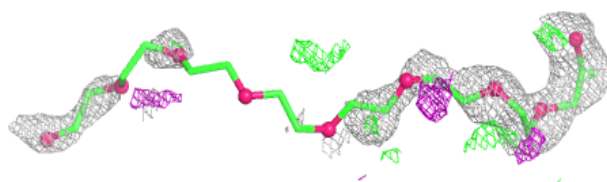
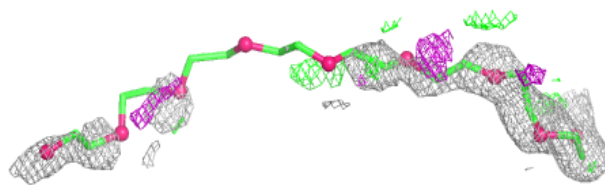
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	P4G	D	308	11/11	0.71	0.28	60,76,82,83	0
9	PE8	D	309	25/25	0.74	0.24	47,73,104,106	0
4	EDO	D	301	4/4	0.78	0.17	46,58,59,63	0
6	SO4	A	305	5/5	0.78	0.18	96,96,100,119	0
5	GOL	D	306	6/6	0.80	0.18	65,72,73,76	0
4	EDO	D	302	4/4	0.81	0.17	70,73,76,77	0
6	SO4	A	306	5/5	0.81	0.14	113,115,126,130	0
8	P4G	C	102	11/11	0.84	0.20	57,64,70,71	0
5	GOL	E	305	6/6	0.85	0.21	56,64,67,70	0
4	EDO	B	102	4/4	0.86	0.15	39,41,41,47	0
5	GOL	A	303	6/6	0.86	0.18	75,77,77,78	0
6	SO4	A	304	5/5	0.86	0.12	82,85,94,95	0
5	GOL	D	304	6/6	0.86	0.13	47,61,64,70	0
4	EDO	E	304	4/4	0.87	0.20	47,54,55,57	0
6	SO4	D	307	5/5	0.88	0.12	93,94,97,111	0
5	GOL	D	305	6/6	0.88	0.13	38,45,53,56	0
5	GOL	D	303	6/6	0.90	0.12	55,57,61,62	0
4	EDO	E	302	4/4	0.90	0.13	37,40,45,49	0
4	EDO	E	303	4/4	0.91	0.12	35,38,42,42	0
4	EDO	A	302	4/4	0.92	0.10	46,47,49,51	0
7	NA	B	101	1/1	0.93	0.07	51,51,51,51	0
4	EDO	B	103	4/4	0.93	0.12	35,38,39,44	0
4	EDO	A	301	4/4	0.94	0.09	37,38,41,47	0
4	EDO	C	101	4/4	0.95	0.07	33,34,34,35	0
10	CA	E	301	1/1	0.95	0.16	65,65,65,65	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 PE8 D 309:

$2mF_o-DF_c$ (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.