



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:22 am BST

PDB ID : 4JIJ
Title : Crystal structure of an inactive mutant of MMP-9 catalytic domain in complex with a fluorogenic synthetic peptidic substrate
Authors : Stura, E.A.; Vera, L.; Cassar-Lajeunesse, E.; Tranchant, I.; Amoura, M.; Dive, V.
Deposited on : 2013-03-06
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

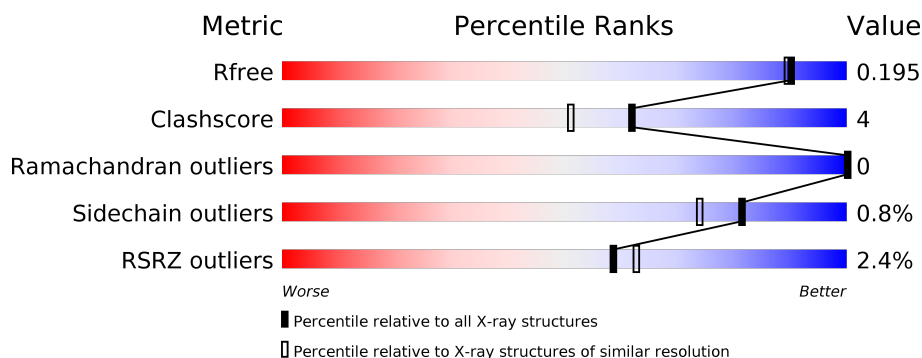
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	P	9	<div> <div></div> <div>78%22%</div> </div>
1	Q	9	<div> <div>11%</div> <div>78%22%</div> </div>
2	A	164	<div> <div></div> <div>92%8%</div> </div>
2	B	164	<div> <div>4%</div> <div>96%</div> <div>..</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 3370 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 fluorogenic peptidic substrate (8MC)PLG(PHI)(DNW)AR(NH₂).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	9	Total	C	I	N	O	0	0	1
			82	52	1	14	15			
1	Q	9	Total	C	I	N	O	0	0	1
			82	52	1	14	15			

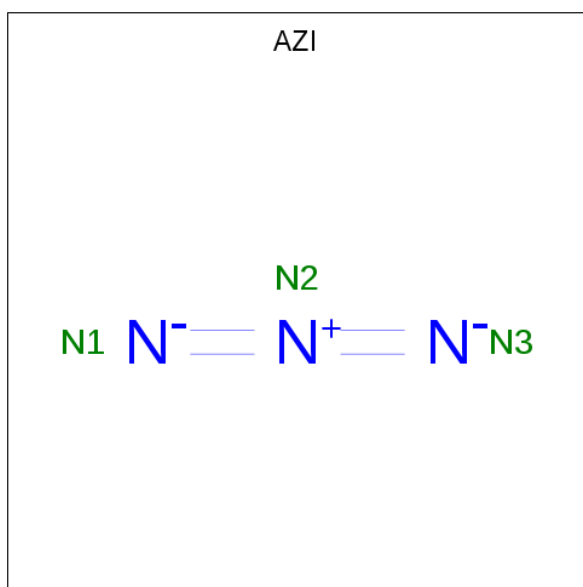
- Molecule 2 is a protein called Matrix metalloproteinase-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	164	Total	C	N	O	S	0	9	0
			1378	886	235	255	2			
2	B	164	Total	C	N	O	S	0	5	0
			1342	865	229	246	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	ALA	GLU	ENGINEERED MUTATION	UNP P14780
B	227	ALA	GLU	ENGINEERED MUTATION	UNP P14780

- Molecule 3 is AZIDE ION (three-letter code: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 3 3	0	0
3	Q	1	Total N 3 3	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Zn 2 2	0	0
4	A	2	Total Zn 2 2	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	A	1	Total Ca 1 1	0	0

- Molecule 6 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

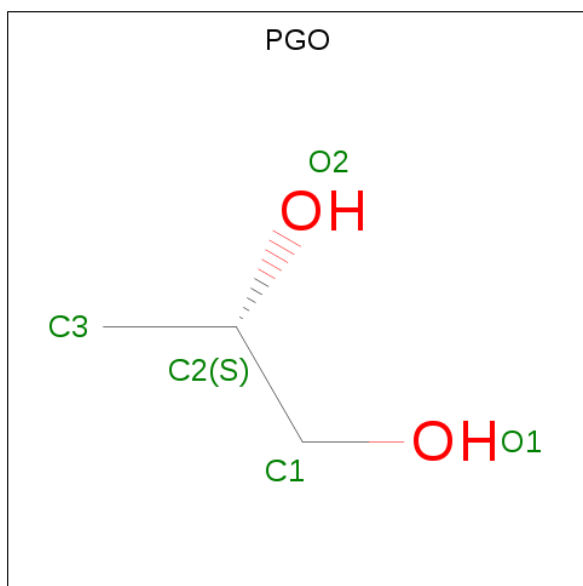
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Sr 2 2	0	0

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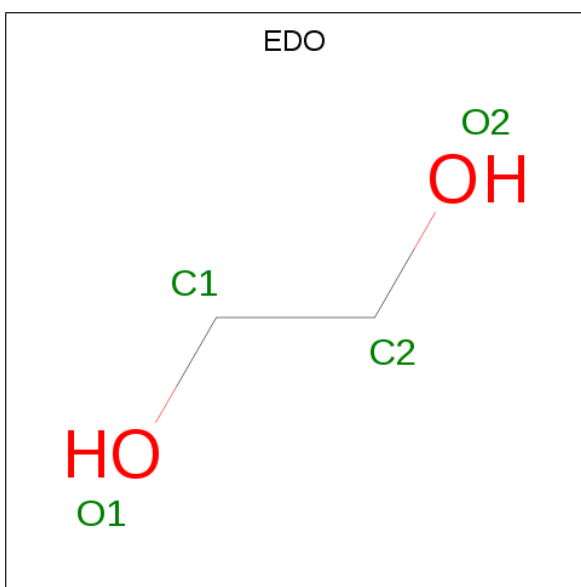
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Sr	0	0
			2	2		

- Molecule 7 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



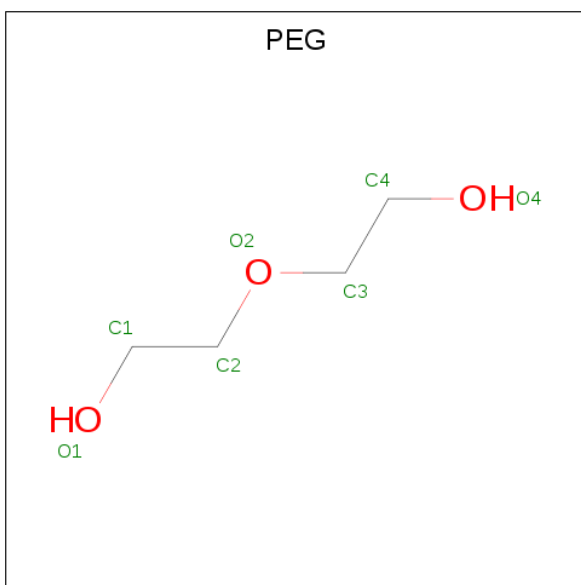
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			5	3	2		
7	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



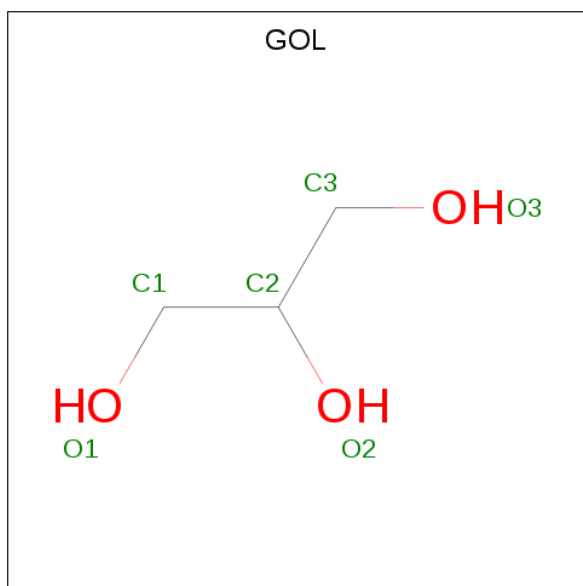
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	1
			12	6	6		
10	B	1	Total	C	O	0	0
			6	3	3		


- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	P	14	Total	O	0	0
			14	14		
11	A	188	Total	O	0	7
			190	190		
11	Q	8	Total	O	0	0
			8	8		
11	B	200	Total	O	0	10
			207	207		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

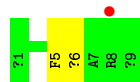
- Molecule 1: fluorogenic peptidic substrate (8MC)PLG(PHI)(DNW)AR(NH2)

Chain P: 



- Molecule 1: fluorogenic peptidic substrate (8MC)PLG(PHI)(DNW)AR(NH2)

Chain Q: 



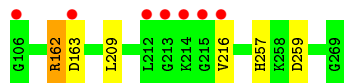
- Molecule 2: Matrix metalloproteinase-9

Chain A: 



- Molecule 2: Matrix metalloproteinase-9

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	34.20Å 57.40Å 172.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.57 – 1.70 40.57 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.57-1.70) 99.8 (40.57-1.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.160 , 0.195 0.161 , 0.195	Depositor DCC
R_{free} test set	1922 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3370	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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: AZI, PHI, GOL, PGO, CA, NH2, ZN, 8MC, DNW, EDO, PEG, SR

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	P	0.27	0/34	0.46	0/42
1	Q	0.25	0/34	0.43	0/42
2	A	0.36	0/1427	0.52	0/1944
2	B	0.34	0/1391	0.51	0/1895
All	All	0.35	0/2886	0.51	0/3923

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	82	0	62	2	0
1	Q	82	0	62	3	0
2	A	1378	0	1255	14	0
2	B	1342	0	1231	5	0
3	A	3	0	0	0	0
3	Q	3	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	5	0	6	0	0
7	B	5	0	6	0	0
8	A	8	0	12	0	0
8	B	8	0	12	1	0
9	A	7	0	10	1	0
10	A	12	0	16	0	0
10	B	6	0	8	0	0
11	A	190	0	0	4	0
11	B	207	0	0	4	0
11	P	14	0	0	0	0
11	Q	8	0	0	0	0
All	All	3370	0	2680	25	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (25) 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:P:5:PHI:I	11:A:417:HOH:O	2.40	1.07
2:A:251[B]:THR:HG22	2:A:253:GLY:H	1.42	0.82
2:A:257[B]:HIS:CD2	2:A:259:ASP:H	1.97	0.82
2:A:257[B]:HIS:HD2	2:A:259:ASP:H	1.28	0.82
2:B:257[B]:HIS:HD2	2:B:259:ASP:H	1.28	0.81
2:B:257[B]:HIS:CD2	2:B:259:ASP:H	2.00	0.80
1:Q:5:PHI:I	11:B:434:HOH:O	2.71	0.79
2:A:134[B]:ARG:HG3	2:A:134[B]:ARG:HH11	1.58	0.68
2:A:241[B]:GLU:HB2	11:A:485[B]:HOH:O	2.02	0.59
2:A:174[B]:GLU:CD	2:A:174[B]:GLU:H	2.06	0.59
2:A:115:LYS:HD2	2:A:117:HIS:CE1	2.43	0.53
2:A:134[B]:ARG:NH2	11:A:522:HOH:O	2.35	0.52
2:A:248:TYR:HE2	9:A:310:PEG:H22	1.75	0.52
1:Q:6:DNW:O32	1:Q:6:DNW:N13	2.42	0.51
2:A:241[A]:GLU:HB2	2:A:257[A]:HIS:CE1	2.48	0.49
2:B:162[A]:ARG:NH2	11:B:550:HOH:O	2.28	0.48
2:B:162[B]:ARG:NH2	11:B:456:HOH:O	2.42	0.47
2:B:209:LEU:HD23	2:B:216:VAL:HG22	1.97	0.46
2:A:134[B]:ARG:CG	2:A:134[B]:ARG:HH11	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:308:EDO:H12	11:B:592:HOH:O	2.17	0.44
2:A:251[B]:THR:HG21	11:A:553:HOH:O	2.17	0.43
2:A:235[B]:ASP:OD1	2:A:236:HIS:N	2.50	0.42
1:P:6:DNW:H5	1:P:6:DNW:H10	1.83	0.41
2:A:264:ILE:HA	2:A:264:ILE:HD12	1.98	0.41
1:Q:6:DNW:H5	1:Q:6:DNW:H10	1.73	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	P	5/9 (56%)	5 (100%)	0	0	100	100
1	Q	5/9 (56%)	5 (100%)	0	0	100	100
2	A	171/164 (104%)	167 (98%)	4 (2%)	0	100	100
2	B	167/164 (102%)	162 (97%)	5 (3%)	0	100	100
All	All	348/346 (101%)	339 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	3/3 (100%)	3 (100%)	0	100	100
1	Q	3/3 (100%)	3 (100%)	0	100	100
2	A	139/130 (107%)	139 (100%)	0	100	100
2	B	135/130 (104%)	131 (97%)	4 (3%)	41	22
All	All	280/266 (105%)	276 (99%)	4 (1%)	81	53

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	162[A]	ARG
2	B	162[B]	ARG
2	B	163[A]	ASP
2	B	163[B]	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PHI	P	5	1	11,12,13	0.86	0	12,15,17	1.49	1 (8%)
1	DNW	Q	6	1	14,18,19	1.11	1 (7%)	12,24,26	1.29	2 (16%)
1	PHI	Q	5	1	11,12,13	0.89	0	12,15,17	1.56	2 (16%)
1	DNW	P	6	1	14,18,19	1.11	1 (7%)	12,24,26	1.23	1 (8%)

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
1	PHI	P	5	1	-	3/5/6/8	0/1/1/1
1	DNW	Q	6	1	-	0/8/15/17	0/1/1/1
1	PHI	Q	5	1	-	3/5/6/8	0/1/1/1
1	DNW	P	6	1	-	0/8/15/17	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	6	DNW	C3-N3	-3.01	1.40	1.45
1	P	6	DNW	C3-N3	-2.99	1.40	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	5	PHI	CG-CB-CA	4.60	123.42	114.10
1	P	5	PHI	CG-CB-CA	4.29	122.79	114.10
1	P	6	DNW	C6-C5-N5	2.93	121.58	119.38
1	Q	6	DNW	C6-C5-N5	2.60	121.33	119.38
1	Q	6	DNW	C3-C2-N13	-2.19	119.48	123.33
1	Q	5	PHI	CB-CA-C	-2.17	107.39	111.47

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Q	5	PHI	C-CA-CB-CG
1	Q	5	PHI	CA-CB-CG-CD2
1	P	5	PHI	CA-CB-CG-CD2
1	Q	5	PHI	CA-CB-CG-CD1
1	P	5	PHI	CA-CB-CG-CD1
1	P	5	PHI	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	5	PHI	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Q	6	DNW	2	0
1	Q	5	PHI	1	0
1	P	6	DNW	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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	$\# Z > 2$
8	EDO	A	308	-	3,3,3	0.45	0	2,2,2	0.37	0
7	PGO	A	307	6	3,4,4	0.21	0	1,4,4	0.05	0
8	EDO	A	309	-	3,3,3	0.46	0	2,2,2	0.34	0
3	AZI	A	301	4	0,2,2	0.00	-	0,1,1	0.00	-
7	PGO	B	306	6	3,4,4	0.40	0	1,4,4	0.19	0
8	EDO	B	307	-	3,3,3	0.47	0	2,2,2	0.41	0
10	GOL	A	311[B]	-	5,5,5	0.39	0	5,5,5	0.30	0
8	EDO	B	308	-	3,3,3	0.22	0	2,2,2	0.15	0
3	AZI	Q	101	4	0,2,2	0.00	-	0,1,1	0.00	-
10	GOL	A	311[A]	-	5,5,5	0.40	0	5,5,5	0.14	0
10	GOL	B	309	-	5,5,5	0.36	0	5,5,5	0.20	0
9	PEG	A	310	-	6,6,6	0.61	0	5,5,5	1.45	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
8	EDO	A	308	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGO	A	307	6	-	1/2/2/2	-
8	EDO	A	309	-	-	0/1/1/1	-
7	PGO	B	306	6	-	2/2/2/2	-
8	EDO	B	307	-	-	0/1/1/1	-
10	GOL	A	311[B]	-	-	4/4/4/4	-
8	EDO	B	308	-	-	0/1/1/1	-
10	GOL	A	311[A]	-	-	2/4/4/4	-
10	GOL	B	309	-	-	2/4/4/4	-
9	PEG	A	310	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	306	PGO	O1-C1-C2-C3
7	B	306	PGO	O1-C1-C2-O2
10	A	311[B]	GOL	C1-C2-C3-O3
10	B	309	GOL	O1-C1-C2-C3
9	A	310	PEG	O1-C1-C2-O2
10	A	311[B]	GOL	O1-C1-C2-C3
10	A	311[A]	GOL	O1-C1-C2-C3
10	A	311[A]	GOL	O1-C1-C2-O2
10	B	309	GOL	O1-C1-C2-O2
10	A	311[B]	GOL	O2-C2-C3-O3
10	A	311[B]	GOL	O1-C1-C2-O2
9	A	310	PEG	C1-C2-O2-C3
7	A	307	PGO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	308	EDO	1	0
9	A	310	PEG	1	0

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	P	5/9 (55%)	-0.23	0 100 100	13, 13, 20, 42	0
1	Q	5/9 (55%)	0.39	1 (20%) 1 0	15, 17, 24, 41	0
2	A	164/164 (100%)	-0.36	0 100 100	8, 13, 27, 41	0
2	B	164/164 (100%)	-0.16	7 (4%) 35 39	9, 15, 34, 51	0
All	All	338/346 (97%)	-0.25	8 (2%) 59 63	8, 15, 31, 51	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	106	GLY	5.1
2	B	214	LYS	4.3
2	B	213	GLY	3.8
1	Q	8	ARG	2.4
2	B	215	GLY	2.4
2	B	163[A]	ASP	2.3
2	B	216	VAL	2.3
2	B	212	LEU	2.0

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

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
1	DNW	Q	6	18/19	0.91	0.13	14,21,33,39	0
1	DNW	P	6	18/19	0.91	0.11	11,18,32,36	0
1	PHI	Q	5	12/13	0.99	0.07	13,14,16,23	0
1	PHI	P	5	12/13	0.99	0.05	11,12,15,21	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	EDO	B	308	4/4	0.68	0.33	42,44,46,54	0
8	EDO	B	307	4/4	0.68	0.19	35,40,40,42	0
8	EDO	A	308	4/4	0.80	0.24	33,39,40,41	0
10	GOL	A	311[B]	6/6	0.80	0.30	30,32,35,37	6
10	GOL	A	311[A]	6/6	0.80	0.30	29,32,35,37	6
10	GOL	B	309	6/6	0.81	0.35	35,41,46,50	0
9	PEG	A	310	7/7	0.82	0.24	30,33,42,52	0
7	PGO	B	306	5/5	0.91	0.12	19,20,25,25	0
7	PGO	A	307	5/5	0.92	0.17	16,22,26,33	0
3	AZI	Q	101	3/3	0.96	0.15	15,15,18,19	0
8	EDO	A	309	4/4	0.97	0.06	16,17,27,34	0
3	AZI	A	301	3/3	0.97	0.19	13,13,14,15	0
5	CA	B	303	1/1	0.99	0.03	13,13,13,13	0
4	ZN	A	302	1/1	1.00	0.05	11,11,11,11	0
6	SR	A	305	1/1	1.00	0.03	14,14,14,14	0
4	ZN	B	302	1/1	1.00	0.04	14,14,14,14	0
5	CA	A	304	1/1	1.00	0.04	10,10,10,10	0
6	SR	B	304	1/1	1.00	0.02	17,17,17,17	0
4	ZN	A	303	1/1	1.00	0.06	10,10,10,10	0
6	SR	A	306	1/1	1.00	0.05	20,20,20,20	0
4	ZN	B	301	1/1	1.00	0.04	12,12,12,12	0
6	SR	B	305	1/1	1.00	0.03	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.