



wwPDB X-ray Structure Validation Summary Report

Oct 9, 2023 – 03:29 PM EDT

PDB ID : 8DRU
Title : Product structure of SARS-CoV-2 Mpro C145A mutant in complex with nsp7-nsp8 (C7) cut site sequence
Authors : Lee, J.; Kenward, C.; Worrall, L.J.; Vuckovic, M.; Paetzel, M.; Strynadka, N.C.J.
Deposited on : 2022-07-21
Resolution : 2.31 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

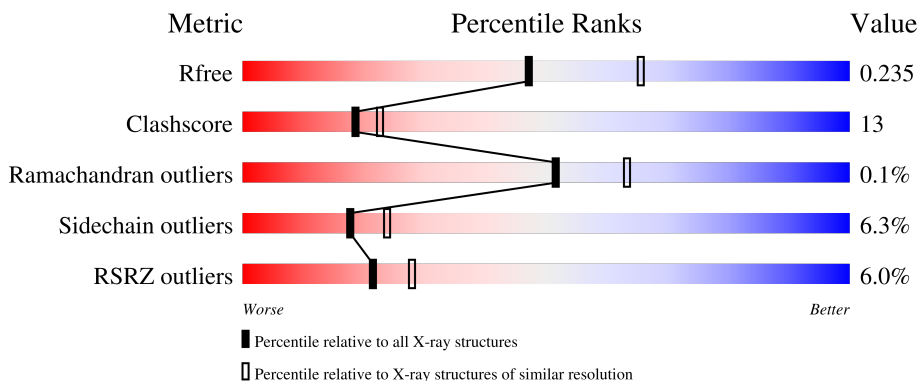
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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.



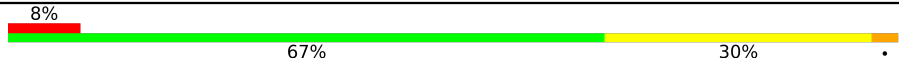

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	306	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">9% 71% 27% •</p>
1	B	306	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 85% 14% •</p>
1	C	306	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 72% 26% •</p>
1	D	306	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8% 71% 25% 5% •</p>
1	E	306	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 76% 23% •</p>

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Mol	Chain	Length	Quality of chain
1	F	306	
1	G	306	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16871 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.

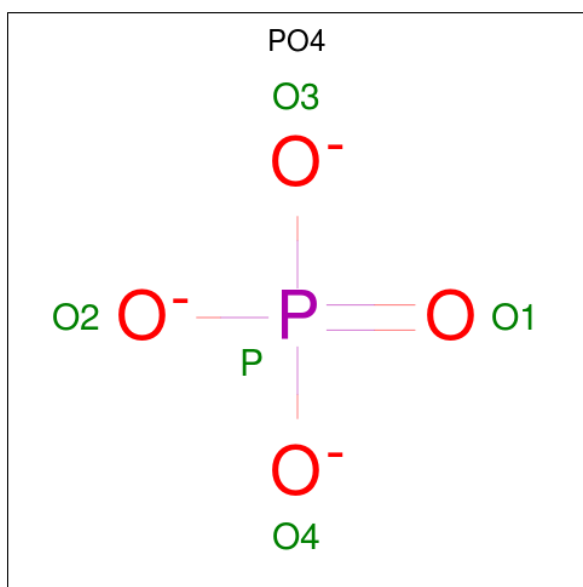
- Molecule 1 is a protein called Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2334	1471	398	444	21	0	0	0
1	B	306	2367	1497	406	443	21	0	0	0
1	C	306	2377	1501	410	445	21	0	2	0
1	D	306	2356	1489	404	443	20	0	0	0
1	E	306	2358	1490	403	444	21	0	0	0
1	F	306	2342	1478	401	442	21	0	1	0
1	G	306	2364	1494	403	446	21	0	2	0

There are 7 discrepancies between the modelled and reference sequences:

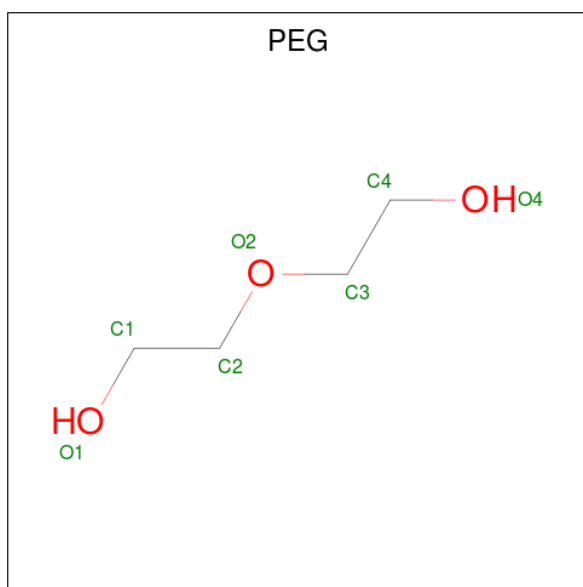
Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ALA	CYS	engineered mutation	UNP P0DTD1
B	145	ALA	CYS	engineered mutation	UNP P0DTD1
C	145	ALA	CYS	engineered mutation	UNP P0DTD1
D	145	ALA	CYS	engineered mutation	UNP P0DTD1
E	145	ALA	CYS	engineered mutation	UNP P0DTD1
F	145	ALA	CYS	engineered mutation	UNP P0DTD1
G	145	ALA	CYS	engineered mutation	UNP P0DTD1

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



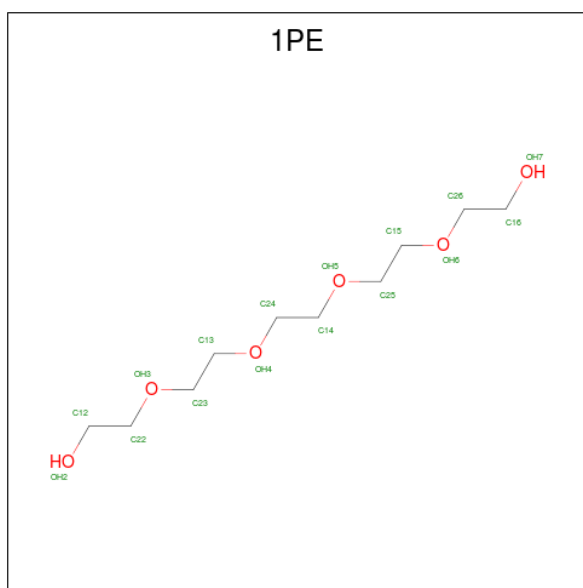
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	G	1	Total C O 7 4 3	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	E	1	Total	C	O	0	0
			14	8	6		
4	G	1	Total	C	O	0	0
			16	10	6		

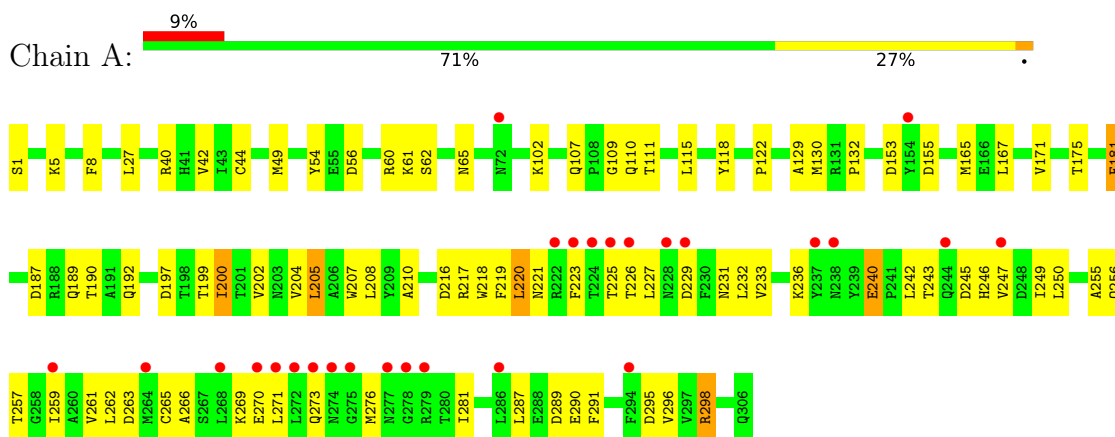
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		
5	B	48	Total	O	0	0
			48	48		
5	C	49	Total	O	0	0
			49	49		
5	D	18	Total	O	0	0
			18	18		
5	E	18	Total	O	0	0
			18	18		
5	F	12	Total	O	0	0
			12	12		
5	G	19	Total	O	0	0
			19	19		

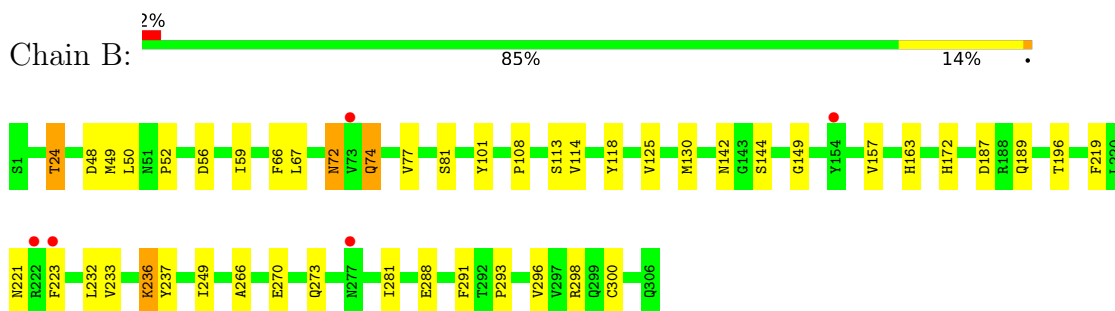
3 Residue-property plots [i](#)

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

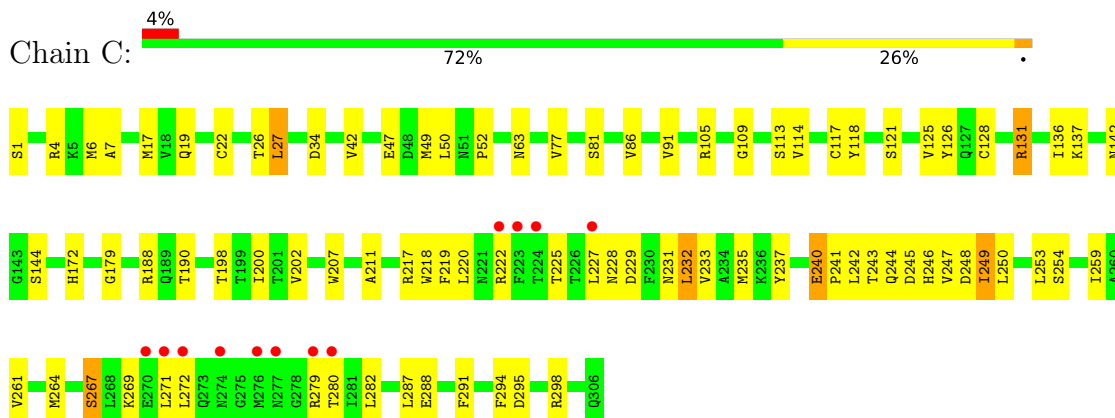
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



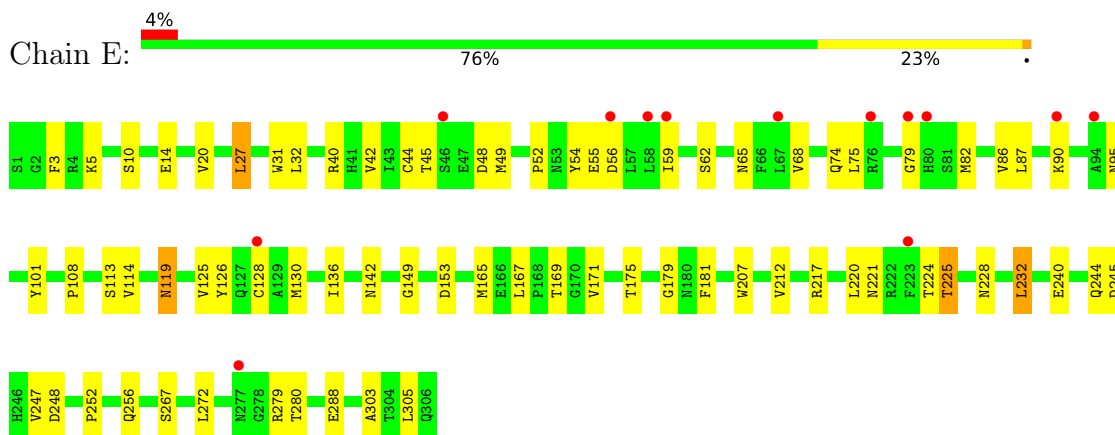
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



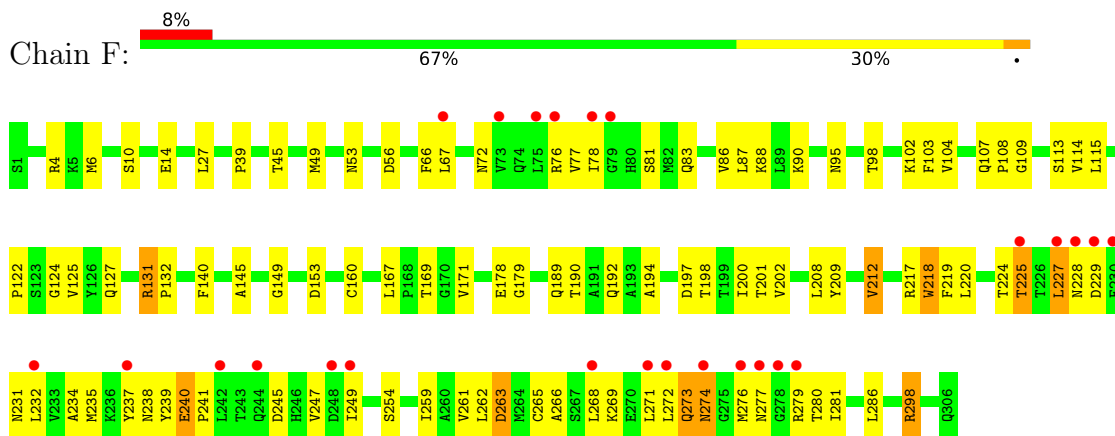
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



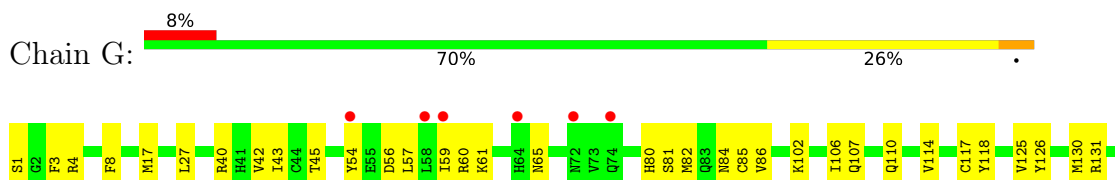
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site

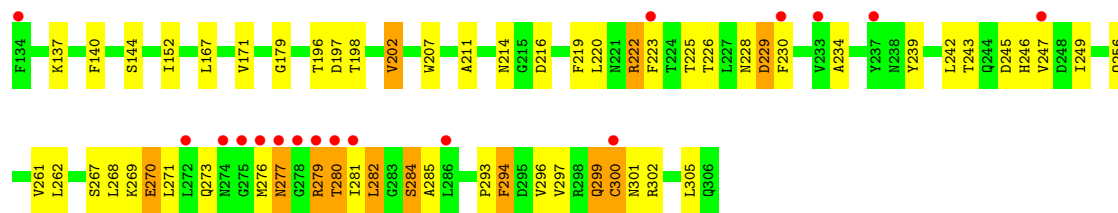


- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.11Å 174.89Å 96.33Å 90.00° 106.34° 90.00°	Depositor
Resolution (Å)	46.22 – 2.31 46.22 – 2.31	Depositor EDS
% Data completeness (in resolution range)	70.3 (46.22-2.31) 70.3 (46.22-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.32Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.190 , 0.237 0.189 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtrriage
Anisotropy	0.007	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16871	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: PO4, PEG, 1PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/2383	0.70	0/3243
1	B	0.47	0/2419	0.64	0/3287
1	C	0.50	0/2434	0.69	0/3306
1	D	0.49	0/2408	0.68	0/3274
1	E	0.46	0/2409	0.63	0/3274
1	F	0.48	0/2395	0.69	0/3259
1	G	0.50	1/2422 (0.0%)	0.69	0/3294
All	All	0.49	1/16870 (0.0%)	0.67	0/22937

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	293	PRO	C-N	5.27	1.46	1.34

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	A	2334	0	2265	80	0
1	B	2367	0	2319	30	0
1	C	2377	0	2335	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2356	0	2287	72	0
1	E	2358	0	2305	51	0
1	F	2342	0	2274	78	0
1	G	2364	0	2298	73	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
3	A	28	0	40	6	0
3	B	14	0	20	0	0
3	C	21	0	30	1	0
3	D	7	0	10	0	0
3	E	7	0	10	2	0
3	F	14	0	20	3	0
3	G	7	0	10	0	0
4	E	14	0	17	1	0
4	G	16	0	22	0	0
5	A	41	0	0	1	0
5	B	48	0	0	0	0
5	C	49	0	0	1	0
5	D	18	0	0	2	0
5	E	18	0	0	0	0
5	F	12	0	0	0	1
5	G	19	0	0	1	0
All	All	16871	0	16262	433	1

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 13.

The worst 5 of 433 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:G:40:ARG:HH11	1:G:82:MET:CE	1.63	1.11
1:C:27:LEU:HD21	1:C:42:VAL:HB	1.34	1.03
1:A:217:ARG:HB3	1:A:220:LEU:HD12	1.32	1.03
1:G:106:ILE:HD11	1:G:130:MET:HE1	1.43	1.01
1:G:40:ARG:HH11	1:G:82:MET:HE2	1.25	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:512:HOH:O	5:F:512:HOH:O[2_555]	2.11	0.09

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	304/306 (99%)	289 (95%)	14 (5%)	1 (0%)	41	50
1	B	304/306 (99%)	299 (98%)	5 (2%)	0	100	100
1	C	306/306 (100%)	292 (95%)	14 (5%)	0	100	100
1	D	304/306 (99%)	293 (96%)	10 (3%)	1 (0%)	41	50
1	E	304/306 (99%)	291 (96%)	13 (4%)	0	100	100
1	F	305/306 (100%)	289 (95%)	16 (5%)	0	100	100
1	G	306/306 (100%)	286 (94%)	20 (6%)	0	100	100
All	All	2133/2142 (100%)	2039 (96%)	92 (4%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	D	154	TYR

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	A	255/262 (97%)	241 (94%)	14 (6%)	21	29
1	B	261/262 (100%)	253 (97%)	8 (3%)	40	55
1	C	263/262 (100%)	246 (94%)	17 (6%)	17	22
1	D	257/262 (98%)	239 (93%)	18 (7%)	15	19
1	E	260/262 (99%)	252 (97%)	8 (3%)	40	55
1	F	256/262 (98%)	233 (91%)	23 (9%)	9	11
1	G	260/262 (99%)	232 (89%)	28 (11%)	6	7
All	All	1812/1834 (99%)	1696 (94%)	116 (6%)	18	23

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	PHE
1	G	294	PHE
1	F	178	GLU
1	G	284	SER
1	G	229	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	127	GLN
1	G	301	ASN
1	E	119	ASN
1	G	19	GLN
1	E	65	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	C	401	-	4,4,4	0.51	0	6,6,6	1.06	0
3	PEG	C	403	-	6,6,6	0.10	0	5,5,5	0.08	0
2	PO4	B	401	-	4,4,4	0.76	0	6,6,6	0.80	0
3	PEG	A	404	-	6,6,6	0.38	0	5,5,5	0.16	0
3	PEG	E	402	-	6,6,6	0.20	0	5,5,5	0.11	0
4	1PE	G	403	-	15,15,15	0.14	0	14,14,14	0.13	0
4	1PE	E	403	-	12,12,15	0.34	0	11,11,14	0.27	0
3	PEG	B	404	-	6,6,6	0.12	0	5,5,5	0.08	0
3	PEG	B	403	-	6,6,6	0.28	0	5,5,5	0.14	0
3	PEG	C	402	-	6,6,6	0.10	0	5,5,5	0.11	0
2	PO4	G	401	-	4,4,4	0.69	0	6,6,6	0.42	0
3	PEG	A	402	-	6,6,6	0.18	0	5,5,5	0.22	0
2	PO4	F	401	-	4,4,4	0.68	0	6,6,6	0.42	0
3	PEG	F	403	-	6,6,6	0.09	0	5,5,5	0.11	0
2	PO4	D	401	-	4,4,4	0.61	0	6,6,6	0.66	0
2	PO4	E	401	-	4,4,4	0.66	0	6,6,6	0.95	0
3	PEG	F	402	-	6,6,6	0.09	0	5,5,5	0.09	0
3	PEG	G	402	-	6,6,6	0.21	0	5,5,5	0.07	0
3	PEG	C	404	-	6,6,6	0.09	0	5,5,5	0.12	0
2	PO4	A	401	-	4,4,4	0.71	0	6,6,6	0.76	0
3	PEG	A	403	-	6,6,6	0.38	0	5,5,5	0.15	0
2	PO4	B	402	-	4,4,4	0.73	0	6,6,6	0.44	0
3	PEG	A	405	-	6,6,6	0.37	0	5,5,5	0.15	0
3	PEG	D	402	-	6,6,6	0.09	0	5,5,5	0.08	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	B	403	-	-	2/4/4/4	-
3	PEG	C	402	-	-	4/4/4/4	-
3	PEG	C	403	-	-	2/4/4/4	-
3	PEG	F	403	-	-	1/4/4/4	-
3	PEG	G	402	-	-	3/4/4/4	-
3	PEG	C	404	-	-	1/4/4/4	-
3	PEG	A	404	-	-	2/4/4/4	-
3	PEG	E	402	-	-	3/4/4/4	-
4	1PE	G	403	-	-	8/13/13/13	-
3	PEG	D	402	-	-	3/4/4/4	-
3	PEG	A	403	-	-	3/4/4/4	-
3	PEG	A	405	-	-	4/4/4/4	-
3	PEG	A	402	-	-	3/4/4/4	-
4	1PE	E	403	-	-	6/10/10/13	-
3	PEG	F	402	-	-	0/4/4/4	-
3	PEG	B	404	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	PEG	O1-C1-C2-O2
3	C	404	PEG	O2-C3-C4-O4
4	G	403	1PE	OH2-C12-C22-OH3
4	G	403	1PE	OH5-C14-C24-OH4
3	C	402	PEG	C4-C3-O2-C2

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	PEG	2	0
3	E	402	PEG	2	0
4	E	403	1PE	1	0
3	C	402	PEG	1	0
3	A	402	PEG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	403	PEG	2	0
2	E	401	PO4	1	0
3	F	402	PEG	1	0
3	A	405	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	306/306 (100%)	0.27	27 (8%) 10 14	28, 51, 122, 149	0
1	B	306/306 (100%)	-0.19	5 (1%) 72 78	31, 47, 77, 128	0
1	C	306/306 (100%)	0.09	12 (3%) 39 46	29, 48, 110, 138	0
1	D	306/306 (100%)	0.17	23 (7%) 14 19	33, 60, 117, 163	0
1	E	306/306 (100%)	0.14	13 (4%) 36 43	35, 63, 104, 148	0
1	F	306/306 (100%)	0.30	25 (8%) 11 15	39, 64, 136, 158	0
1	G	306/306 (100%)	0.28	23 (7%) 14 19	37, 67, 111, 161	0
All	All	2142/2142 (100%)	0.15	128 (5%) 21 28	28, 58, 115, 163	0

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	276	MET	7.5
1	A	247	VAL	7.1
1	G	278	GLY	5.7
1	G	275	GLY	5.1
1	A	223	PHE	5.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	B	404	7/7	0.55	0.29	66,74,86,86	0
3	PEG	A	403	7/7	0.81	0.25	56,60,68,75	0
3	PEG	F	403	7/7	0.81	0.22	72,72,78,84	0
2	PO4	G	401	5/5	0.82	0.23	103,103,122,125	0
3	PEG	B	403	7/7	0.82	0.20	66,70,73,79	0
3	PEG	F	402	7/7	0.84	0.18	63,67,79,80	0
2	PO4	E	401	5/5	0.85	0.13	90,97,105,107	0
3	PEG	C	403	7/7	0.85	0.20	63,72,81,84	0
3	PEG	D	402	7/7	0.88	0.15	61,64,78,88	0
3	PEG	A	405	7/7	0.88	0.17	63,70,74,76	0
3	PEG	C	404	7/7	0.88	0.32	60,67,74,77	0
3	PEG	C	402	7/7	0.89	0.12	56,66,69,70	0
3	PEG	G	402	7/7	0.89	0.16	65,68,74,79	0
3	PEG	A	402	7/7	0.90	0.15	53,56,66,75	0
3	PEG	A	404	7/7	0.90	0.16	54,61,65,66	0
3	PEG	E	402	7/7	0.91	0.23	52,60,66,74	0
4	1PE	G	403	16/16	0.91	0.16	55,59,68,70	0
4	1PE	E	403	14/16	0.92	0.14	47,66,72,77	0
2	PO4	D	401	5/5	0.93	0.12	72,94,101,110	0
2	PO4	F	401	5/5	0.95	0.11	68,68,79,88	0
2	PO4	C	401	5/5	0.95	0.10	64,64,84,87	0
2	PO4	B	402	5/5	0.97	0.16	58,59,65,79	0
2	PO4	A	401	5/5	0.97	0.11	46,58,68,68	0
2	PO4	B	401	5/5	0.98	0.10	57,61,65,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.