



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 02:15 pm BST

PDB ID : 6NYX
Title : Human parainfluenza virus type 3 fusion protein N-terminal heptad repeat domain+VI
Authors : Outlaw, V.K.; Kreitler, D.F.; Gellman, S.H.
Deposited on : 2019-02-12
Resolution : 1.85 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 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

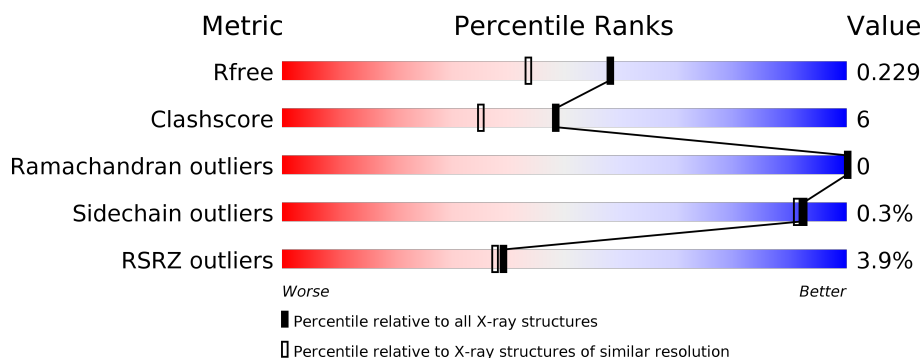
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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.










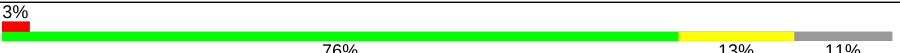
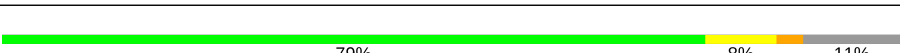
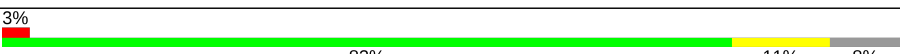
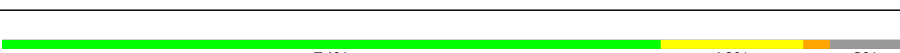
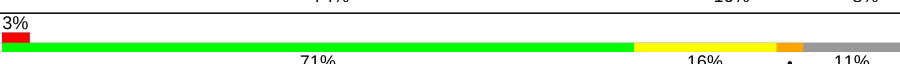
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	A	53	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>13%</div> </div> </div>
1	B	53	<div> <div>9%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>
1	C	53	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>9%</div> </div> </div>
1	D	53	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>8%</div> </div> </div>
1	E	53	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>9%</div> </div> </div>
1	F	53	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	H	53	
1	J	53	
1	L	53	
2	G	38	
2	I	38	
2	K	38	
2	M	38	
2	N	38	
2	O	38	
2	P	38	
2	Q	38	
2	T	38	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12093 atoms, of which 5994 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 glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	46	Total	C	H	N	O	0	0	0
			705	217	357	59	72			
1	B	48	Total	C	H	N	O	0	0	0
			737	226	375	62	74			
1	C	48	Total	C	H	N	O	0	0	0
			704	219	353	61	71			
1	D	49	Total	C	H	N	O	0	0	0
			762	233	389	65	75			
1	E	48	Total	C	H	N	O	0	0	0
			744	227	381	62	74			
1	F	49	Total	C	H	N	O	0	0	0
			753	231	384	63	75			
1	H	51	Total	C	H	N	O	0	0	1
			746	230	378	64	74			
1	J	48	Total	C	H	N	O	0	0	0
			743	227	380	62	74			
1	L	48	Total	C	H	N	O	0	0	0
			749	227	381	66	75			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	ACE	-	acetylation	UNP Q84193
A	190	NH2	-	amidation	UNP Q84193
B	138	ACE	-	acetylation	UNP Q84193
B	190	NH2	-	amidation	UNP Q84193
C	138	ACE	-	acetylation	UNP Q84193
C	190	NH2	-	amidation	UNP Q84193
D	138	ACE	-	acetylation	UNP Q84193
D	190	NH2	-	amidation	UNP Q84193
E	138	ACE	-	acetylation	UNP Q84193
E	190	NH2	-	amidation	UNP Q84193
F	138	ACE	-	acetylation	UNP Q84193

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Chain	Residue	Modelled	Actual	Comment	Reference
F	190	NH2	-	amidation	UNP Q84193
H	138	ACE	-	acetylation	UNP Q84193
H	190	NH2	-	amidation	UNP Q84193
J	138	ACE	-	acetylation	UNP Q84193
J	190	NH2	-	amidation	UNP Q84193
L	138	ACE	-	acetylation	UNP Q84193
L	190	NH2	-	amidation	UNP Q84193

- Molecule 2 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	35	Total	C	H	N	O	0	0	0
			570	177	288	48	57			
2	I	35	Total	C	H	N	O	0	0	0
			583	179	298	49	57			
2	K	35	Total	C	H	N	O	0	0	0
			558	174	279	48	57			
2	M	35	Total	C	H	N	O	0	0	1
			561	173	284	48	56			
2	N	34	Total	C	H	N	O	0	0	0
			555	172	281	48	54			
2	O	34	Total	C	H	N	O	0	0	0
			546	171	274	47	54			
2	P	35	Total	C	H	N	O	0	0	1
			575	176	294	49	56			
2	Q	35	Total	C	H	N	O	0	1	1
			585	181	297	50	57			
2	T	34	Total	C	H	N	O	0	0	0
			573	176	293	48	56			

There are 36 discrepancies between the modelled and reference sequences:

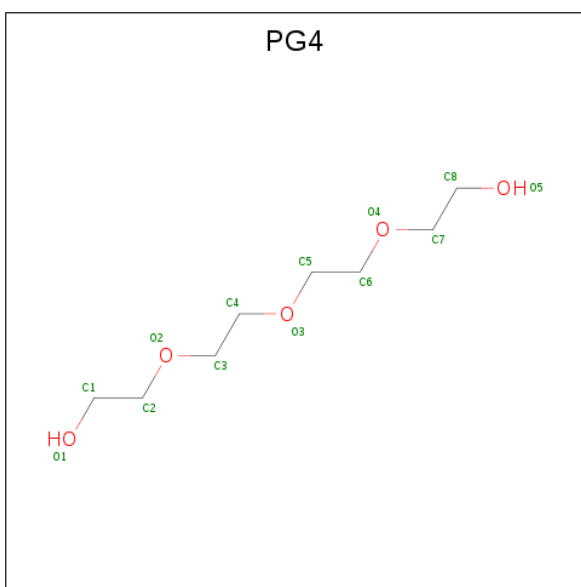
Chain	Residue	Modelled	Actual	Comment	Reference
G	448	ACE	-	acetylation	UNP Q84193
G	459	VAL	GLU	engineered mutation	UNP Q84193
G	463	ILE	ALA	engineered mutation	UNP Q84193
G	485	NH2	-	amidation	UNP Q84193
I	448	ACE	-	acetylation	UNP Q84193
I	459	VAL	GLU	engineered mutation	UNP Q84193
I	463	ILE	ALA	engineered mutation	UNP Q84193
I	485	NH2	-	amidation	UNP Q84193
K	441	ACE	-	acetylation	UNP Q84193

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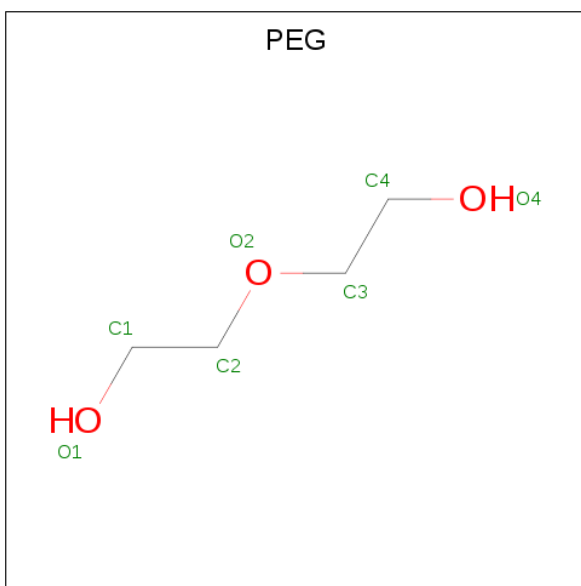
Chain	Residue	Modelled	Actual	Comment	Reference
K	452	VAL	GLU	engineered mutation	UNP Q84193
K	456	ILE	ALA	engineered mutation	UNP Q84193
K	478	NH2	-	amidation	UNP Q84193
M	448	ACE	-	acetylation	UNP Q84193
M	459	VAL	GLU	engineered mutation	UNP Q84193
M	463	ILE	ALA	engineered mutation	UNP Q84193
M	485	NH2	-	amidation	UNP Q84193
N	448	ACE	-	acetylation	UNP Q84193
N	459	VAL	GLU	engineered mutation	UNP Q84193
N	463	ILE	ALA	engineered mutation	UNP Q84193
N	485	NH2	-	amidation	UNP Q84193
O	448	ACE	-	acetylation	UNP Q84193
O	459	VAL	GLU	engineered mutation	UNP Q84193
O	463	ILE	ALA	engineered mutation	UNP Q84193
O	485	NH2	-	amidation	UNP Q84193
P	448	ACE	-	acetylation	UNP Q84193
P	459	VAL	GLU	engineered mutation	UNP Q84193
P	463	ILE	ALA	engineered mutation	UNP Q84193
P	485	NH2	-	amidation	UNP Q84193
Q	448	ACE	-	acetylation	UNP Q84193
Q	459	VAL	GLU	engineered mutation	UNP Q84193
Q	463	ILE	ALA	engineered mutation	UNP Q84193
Q	485	NH2	-	amidation	UNP Q84193
T	448	ACE	-	acetylation	UNP Q84193
T	459	VAL	GLU	engineered mutation	UNP Q84193
T	463	ILE	ALA	engineered mutation	UNP Q84193
T	485	NH2	-	amidation	UNP Q84193

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	14	Total O 14 14	0	0
5	B	17	Total O 17 17	0	0
5	C	15	Total O 15 15	0	0
5	D	14	Total O 14 14	0	0
5	E	14	Total O 14 14	0	0
5	F	20	Total O 21 21	0	1
5	G	19	Total O 19 19	0	0
5	H	17	Total O 17 17	0	0
5	I	19	Total O 19 19	0	0
5	J	15	Total O 15 15	0	0
5	K	14	Total O 14 14	0	0
5	L	12	Total O 12 12	0	0
5	M	17	Total O 17 17	0	0
5	N	29	Total O 29 29	0	0
5	O	15	Total O 15 15	0	0
5	P	20	Total O 21 21	0	1
5	Q	18	Total O 18 18	0	0
5	T	5	Total O 5 5	0	0

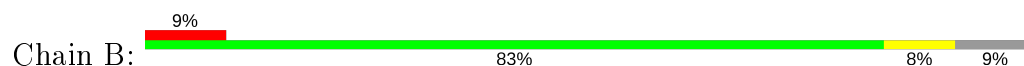
3 Residue-property plots [i](#)

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.

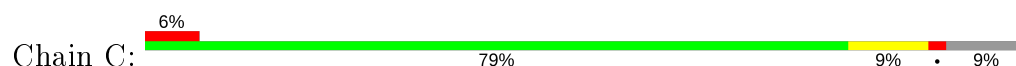
- Molecule 1: Fusion glycoprotein F0



- Molecule 1: Fusion glycoprotein F0



- Molecule 1: Fusion glycoprotein F0



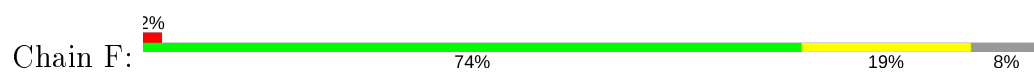
- Molecule 1: Fusion glycoprotein F0



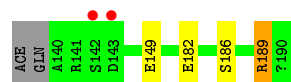
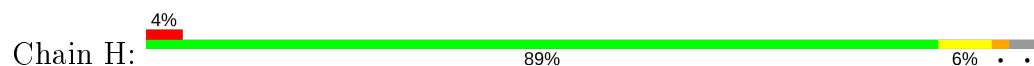
- Molecule 1: Fusion glycoprotein F0



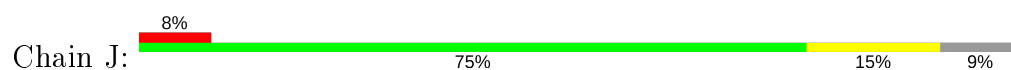
- Molecule 1: Fusion glycoprotein F0



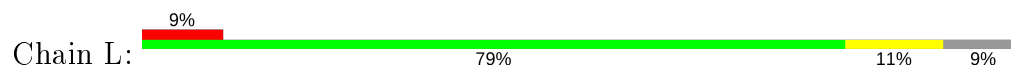
- Molecule 1: Fusion glycoprotein F0



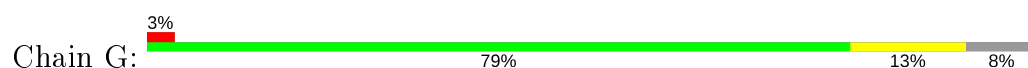
- Molecule 1: Fusion glycoprotein F0



- Molecule 1: Fusion glycoprotein F0



- Molecule 2: Fusion glycoprotein F0



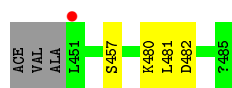
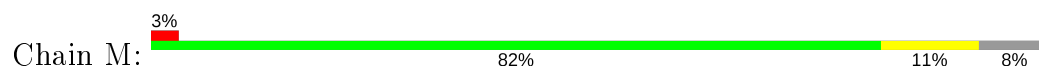
- Molecule 2: Fusion glycoprotein F0



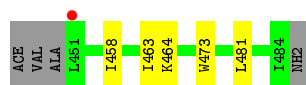
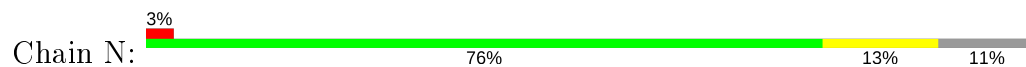
- Molecule 2: Fusion glycoprotein F0



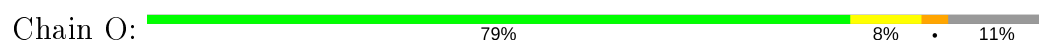
- Molecule 2: Fusion glycoprotein F0



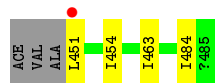
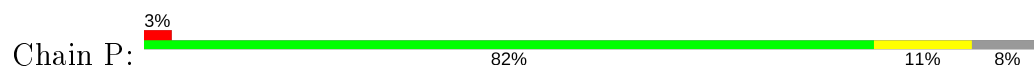
- Molecule 2: Fusion glycoprotein F0



- Molecule 2: Fusion glycoprotein F0



- Molecule 2: Fusion glycoprotein F0



- Molecule 2: Fusion glycoprotein F0



- Molecule 2: Fusion glycoprotein F0



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	88.03Å 88.03Å 75.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.12 – 1.85 38.12 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.12-1.85) 94.2 (38.12-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.198 , 0.229 0.198 , 0.229	Depositor DCC
R_{free} test set	1693 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l 0.013 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12093	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.57% 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: PG4, PEG, NH2

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	0.97	0/349	0.76	0/471
1	B	0.82	0/363	0.79	1/489 (0.2%)
1	C	0.86	0/352	0.71	0/477
1	D	0.71	0/374	0.72	0/504
1	E	0.82	0/364	0.73	0/491
1	F	0.91	0/370	0.63	0/499
1	H	0.97	0/368	0.76	0/498
1	J	0.68	0/364	0.70	0/491
1	L	0.78	0/369	0.72	0/496
2	G	1.00	0/284	0.72	0/382
2	I	0.81	0/287	0.71	0/385
2	K	0.82	0/281	0.74	0/378
2	M	0.94	0/278	0.74	0/374
2	N	0.87	0/276	0.72	0/370
2	O	0.87	0/274	0.72	0/368
2	P	0.91	0/282	0.76	0/378
2	Q	0.97	2/293 (0.7%)	0.92	0/392
2	T	1.04	2/282 (0.7%)	0.74	0/378
All	All	0.88	4/5810 (0.1%)	0.74	1/7821 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	1
2	Q	0	1
2	T	0	2
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	469	GLU	CD-OE1	-6.96	1.18	1.25
2	T	469	GLU	CD-OE2	-6.06	1.19	1.25
2	Q	475[A]	ARG	N-CA	5.32	1.56	1.46
2	Q	475[B]	ARG	N-CA	5.32	1.56	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	ASP	CB-CG-OD2	-5.34	113.49	118.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Sidechain
1	C	152	ARG	Sidechain
1	D	189	ARG	Sidechain
1	E	152	ARG	Sidechain
1	H	189	ARG	Sidechain

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	348	357	357	9	0
1	B	362	375	375	4	0
1	C	351	353	353	6	0
1	D	373	389	388	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	363	381	380	11	0
1	F	369	384	384	12	0
1	H	368	378	376	3	0
1	J	363	380	380	5	2
1	L	368	381	381	3	1
2	G	282	288	288	5	0
2	I	285	298	297	7	2
2	K	279	279	279	0	1
2	M	277	284	281	4	0
2	N	274	281	281	9	0
2	O	272	274	274	4	0
2	P	281	294	292	5	0
2	Q	288	297	299	8	0
2	T	280	293	292	8	0
3	G	13	18	18	1	0
4	L	7	10	10	1	0
5	A	14	0	0	0	0
5	B	17	0	0	0	0
5	C	15	0	0	1	0
5	D	14	0	0	0	0
5	E	14	0	0	0	0
5	F	21	0	0	0	0
5	G	19	0	0	0	0
5	H	17	0	0	0	0
5	I	19	0	0	0	0
5	J	15	0	0	0	0
5	K	14	0	0	0	0
5	L	12	0	0	0	0
5	M	17	0	0	1	1
5	N	29	0	0	0	0
5	O	15	0	0	0	0
5	P	21	0	0	0	0
5	Q	18	0	0	0	1
5	T	5	0	0	0	0
All	All	6099	5994	5985	71	4

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 6.

The worst 5 of 71 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:146:LYS:HE2	2:O:483:SER:OG	1.77	0.84
2:I:476:ARG:O	2:I:480:LYS:HD3	1.85	0.76
1:D:176:GLN:HG3	2:Q:454:ILE:HG23	1.75	0.67
1:E:169:ILE:HG21	2:T:464:LYS:HE2	1.78	0.65
2:N:458:ILE:HD11	2:T:472:GLU:HG3	1.78	0.64

All (4) 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)
2:I:482:ASP:OD1	1:J:152:ARG:HH21[3_555]	1.48	0.12
5:M:501:HOH:O	5:Q:502:HOH:O[3_555]	2.09	0.11
2:I:482:ASP:OD1	1:J:152:ARG:NH2[3_555]	2.13	0.07
2:K:447:ILE:H	1:L:180:ASN:OD1[2_565]	1.60	0.00

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	44/53 (83%)	42 (96%)	2 (4%)	0	100	100
1	B	46/53 (87%)	45 (98%)	1 (2%)	0	100	100
1	C	46/53 (87%)	45 (98%)	1 (2%)	0	100	100
1	D	47/53 (89%)	47 (100%)	0	0	100	100
1	E	46/53 (87%)	46 (100%)	0	0	100	100
1	F	47/53 (89%)	47 (100%)	0	0	100	100
1	H	49/53 (92%)	47 (96%)	2 (4%)	0	100	100
1	J	46/53 (87%)	45 (98%)	1 (2%)	0	100	100
1	L	46/53 (87%)	46 (100%)	0	0	100	100
2	G	33/38 (87%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	33/38 (87%)	33 (100%)	0	0	100	100
2	K	33/38 (87%)	33 (100%)	0	0	100	100
2	M	33/38 (87%)	33 (100%)	0	0	100	100
2	N	32/38 (84%)	32 (100%)	0	0	100	100
2	O	32/38 (84%)	32 (100%)	0	0	100	100
2	P	33/38 (87%)	33 (100%)	0	0	100	100
2	Q	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
2	T	32/38 (84%)	32 (100%)	0	0	100	100
All	All	712/819 (87%)	704 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	40/45 (89%)	40 (100%)	0	100	100
1	B	41/45 (91%)	41 (100%)	0	100	100
1	C	38/45 (84%)	37 (97%)	1 (3%)	46	30
1	D	42/45 (93%)	42 (100%)	0	100	100
1	E	42/45 (93%)	42 (100%)	0	100	100
1	F	42/45 (93%)	42 (100%)	0	100	100
1	H	40/45 (89%)	40 (100%)	0	100	100
1	J	42/45 (93%)	42 (100%)	0	100	100
1	L	42/45 (93%)	42 (100%)	0	100	100
2	G	33/35 (94%)	33 (100%)	0	100	100
2	I	34/35 (97%)	33 (97%)	1 (3%)	42	26
2	K	32/35 (91%)	32 (100%)	0	100	100
2	M	33/35 (94%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	32/35 (91%)	32 (100%)	0	100	100
2	O	31/35 (89%)	31 (100%)	0	100	100
2	P	34/35 (97%)	34 (100%)	0	100	100
2	Q	34/35 (97%)	34 (100%)	0	100	100
2	T	34/35 (97%)	34 (100%)	0	100	100
All	All	666/720 (92%)	664 (100%)	2 (0%)	92	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	152	ARG
2	I	452	ASP

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

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	PG4	G	501	-	12,12,12	0.59	0	11,11,11	0.95	0
4	PEG	L	201	-	6,6,6	0.60	0	5,5,5	0.43	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
3	PG4	G	501	-	-	5/10/10/10	-
4	PEG	L	201	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	501	PG4	O4-C7-C8-O5
3	G	501	PG4	O1-C1-C2-O2
4	L	201	PEG	O2-C3-C4-O4
3	G	501	PG4	C8-C7-O4-C6
4	L	201	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	501	PG4	1	0
4	L	201	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	A	46/53 (86%)	-0.14	1 (2%) 62 61	21, 34, 61, 72	0
1	B	48/53 (90%)	0.30	5 (10%) 6 6	22, 36, 71, 90	0
1	C	48/53 (90%)	0.12	3 (6%) 20 19	21, 42, 68, 70	0
1	D	49/53 (92%)	0.09	1 (2%) 65 64	26, 35, 63, 83	0
1	E	48/53 (90%)	-0.03	1 (2%) 63 63	25, 37, 60, 74	0
1	F	49/53 (92%)	0.01	1 (2%) 65 64	24, 36, 62, 66	0
1	H	50/53 (94%)	0.40	2 (4%) 38 36	22, 36, 85, 96	0
1	J	48/53 (90%)	0.24	4 (8%) 11 11	22, 32, 74, 78	0
1	L	48/53 (90%)	0.24	5 (10%) 6 6	23, 42, 77, 86	0
2	G	35/38 (92%)	0.14	1 (2%) 51 50	24, 35, 70, 75	0
2	I	35/38 (92%)	0.01	1 (2%) 51 50	23, 33, 62, 65	0
2	K	35/38 (92%)	0.13	0 100 100	25, 41, 72, 84	0
2	M	34/38 (89%)	-0.04	1 (2%) 51 50	23, 34, 56, 79	0
2	N	34/38 (89%)	-0.26	1 (2%) 51 50	23, 34, 64, 75	0
2	O	34/38 (89%)	0.03	0 100 100	25, 38, 56, 68	0
2	P	34/38 (89%)	-0.14	1 (2%) 51 50	24, 35, 56, 70	0
2	Q	35/38 (92%)	0.01	0 100 100	26, 36, 60, 68	0
2	T	34/38 (89%)	0.10	1 (2%) 51 50	29, 42, 62, 71	0
All	All	744/819 (90%)	0.08	29 (3%) 39 38	21, 37, 69, 96	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	ALA	6.6
1	L	184	VAL	4.2
1	B	185	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	142	SER	3.7
1	A	185	PRO	3.5

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 carbohydrates 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(\AA^2)	Q<0.9
3	PG4	G	501	13/13	0.60	0.20	47,64,79,87	0
4	PEG	L	201	7/7	0.70	0.37	58,70,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.