



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2021 – 05:30 pm BST

PDB ID : 7AGE  
Title : Protease Sapp1p from Candida parapsilosis in complex with KB32  
Authors : Dostal, J.; Heidingsfeld, O.; Brynda, J.  
Deposited on : 2020-09-22  
Resolution : 1.30 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](mailto: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.

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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 : 2.18  
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) : 2.18

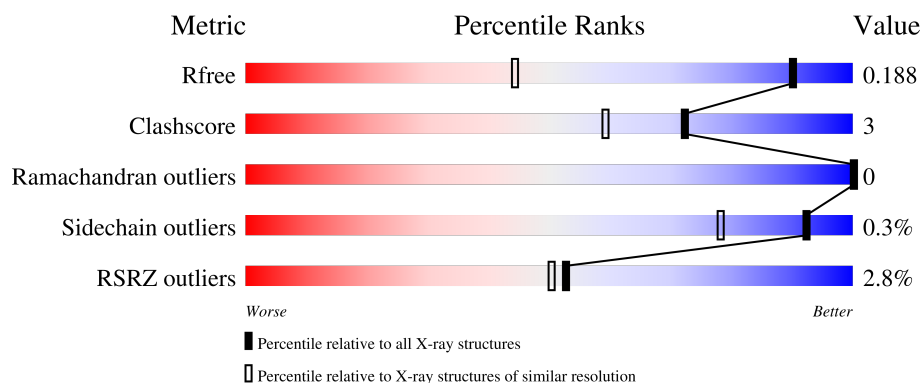
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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  $\geq 3$ , 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	339	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
1	B	339	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
1	D	339	<div> <div>%</div> <div>96%</div> <div>.</div> </div>
1	F	339	<div> <div>3%</div> <div>96%</div> <div>.</div> </div>
2	C	7	<div> <div>57%</div> <div>14%</div> <div>14%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	7	
2	G	7	
2	I	7	

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
3	PEG	B	403	-	-	X	-
3	PEG	D	401	-	-	X	X
3	PEG	D	402	-	-	X	X
3	PEG	D	406	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12278 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 Candidapepsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	12	0
			2579	1609	419	547	4			
1	B	339	Total	C	N	O	S	3	19	0
			2616	1631	426	555	4			
1	D	339	Total	C	N	O	S	0	16	0
			2593	1617	418	554	4			
1	F	339	Total	C	N	O	S	0	20	0
			2618	1636	424	554	4			

- Molecule 2 is a protein called Pepstatin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	0
			52	39	5	8			
2	C	6	Total	C	N	O	0	0	0
			52	39	5	8			
2	E	7	Total	C	N	O	0	0	1
			55	40	6	9			
2	G	6	Total	C	N	O	0	1	0
			64	49	6	9			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

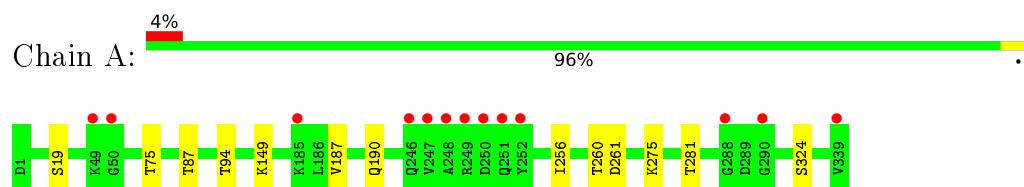
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	356	Total 357	O 357	0	1
4	I	4	Total 4	O 4	0	0
4	B	380	Total 381	O 381	0	1
4	C	4	Total 4	O 4	0	0
4	D	423	Total 426	O 426	0	3
4	E	6	Total 6	O 6	0	0
4	F	380	Total 385	O 385	0	5
4	G	2	Total 2	O 2	0	0

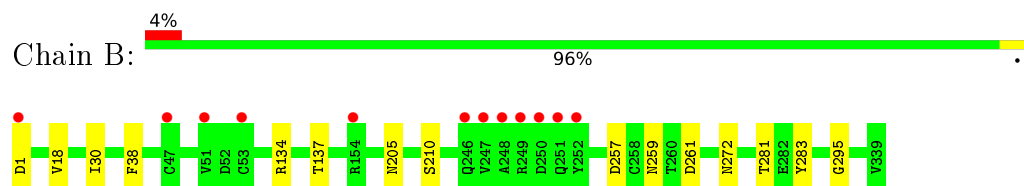
### 3 Residue-property plots [i](#)

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

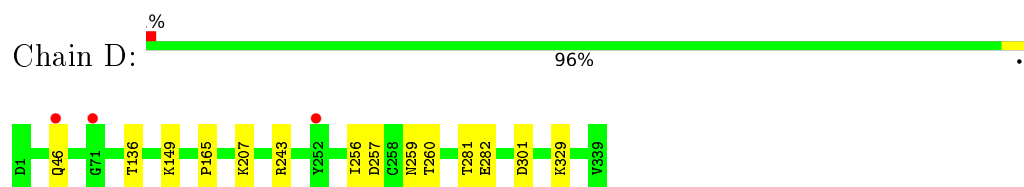
- Molecule 1: Candidapepsin



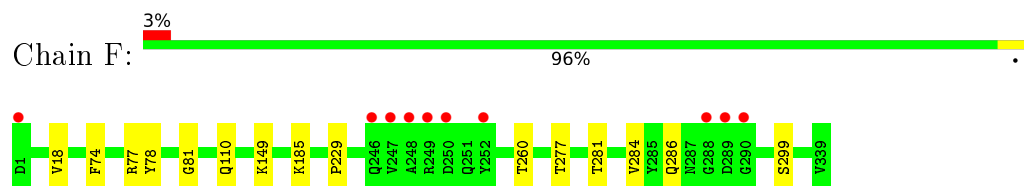
- Molecule 1: Candidapepsin



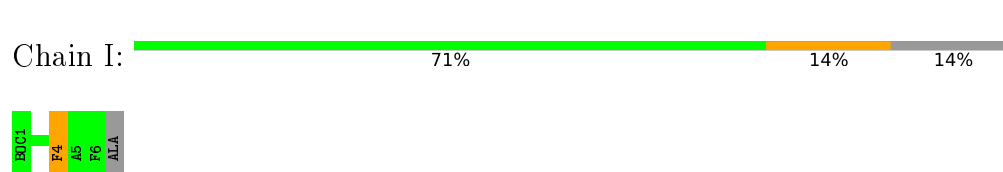
- Molecule 1: Candidapepsin



- Molecule 1: Candidapepsin



- Molecule 2: Pepstatin




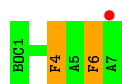
- Molecule 2: Pepstatin

Chain C:  57% 14% 14% 14%



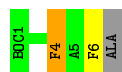
● Molecule 2: Pepstatin

Chain E:  14% 71% 29%



● Molecule 2: Pepstatin

Chain G:  57% 14% 14% 14%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.26 Å 87.29 Å 157.95 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.14 – 1.30 23.14 – 1.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (23.14-1.30) 98.4 (23.14-1.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 1.30 Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.162 , 0.180 0.171 , 0.188	Depositor DCC
$R_{free}$ test set	14594 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6642e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PSA, BOC

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	0.67	0/2656	0.79	1/3615 (0.0%)
1	B	0.64	0/2709	0.78	1/3685 (0.0%)
1	D	0.65	0/2678	0.77	1/3645 (0.0%)
1	F	0.63	0/2722	0.76	0/3705
2	C	1.22	0/17	0.82	0/21
2	E	0.75	0/17	1.06	0/21
2	G	1.05	0/17	0.65	0/21
2	I	1.19	0/17	0.84	0/21
All	All	0.65	0/10833	0.78	3/14734 (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
2	C	0	2
2	E	0	3
2	G	0	2
2	I	0	2
All	All	0	9

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ASP	CB-CG-OD1	5.60	123.34	118.30
1	D	243	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	B	261	ASP	CB-CG-OD1	5.29	123.06	118.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	4	PSA	Mainchain,Peptide
2	E	4	PSA	Mainchain,Peptide
2	E	6	PSA	Mainchain
2	G	4	PSA	Mainchain
2	I	4	PSA	Mainchain,Peptide

## 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	2579	0	2507	14	0
1	B	2616	0	2550	13	0
1	D	2593	0	2515	23	3
1	F	2618	0	2567	16	3
2	C	52	0	54	2	0
2	E	55	0	56	0	0
2	G	64	0	64	0	0
2	I	52	0	54	0	0
3	B	21	0	30	1	7
3	D	42	0	60	16	7
3	F	21	0	30	0	0
4	A	357	0	0	11	4
4	B	381	0	0	7	1
4	C	4	0	0	0	0
4	D	426	0	0	11	2
4	E	6	0	0	0	0
4	F	385	0	0	10	1
4	G	2	0	0	0	0
4	I	4	0	0	0	0
All	All	12278	0	10487	72	15

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 3.

The worst 5 of 72 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:D:257[B]:ASP:OD2	1:D:259[B]:ASN:OD1	1.61	1.19
1:D:281[A]:THR:HG23	3:D:402:PEG:H11	1.36	1.03
1:B:137[A]:THR:OG1	4:B:501:HOH:O	1.77	1.01
1:D:257[B]:ASP:CG	1:D:259[B]:ASN:OD1	2.03	0.97
1:D:281[A]:THR:HG23	3:D:402:PEG:C1	1.97	0.95

The worst 5 of 15 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)
3:B:403:PEG:O2	3:D:401:PEG:O1[4_566]	1.01	1.19
3:B:403:PEG:O2	3:D:401:PEG:C1[4_566]	1.07	1.13
3:B:403:PEG:C2	3:D:401:PEG:C1[4_566]	1.21	0.99
3:B:403:PEG:C1	3:D:401:PEG:C2[4_566]	1.26	0.94
1:D:46:GLN:NE2	1:F:77[B]:ARG:CZ[3_746]	1.54	0.66

## 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	349/339 (103%)	344 (99%)	5 (1%)	0	100	100
1	B	355/339 (105%)	349 (98%)	6 (2%)	0	100	100
1	D	353/339 (104%)	347 (98%)	6 (2%)	0	100	100
1	F	357/339 (105%)	351 (98%)	6 (2%)	0	100	100
2	C	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	E	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	G	3/7 (43%)	3 (100%)	0	0	100	100
2	I	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
All	All	1426/1384 (103%)	1400 (98%)	26 (2%)	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	293/281 (104%)	293 (100%)	0	100	100
1	B	299/281 (106%)	298 (100%)	1 (0%)	92	78
1	D	295/281 (105%)	295 (100%)	0	100	100
1	F	301/281 (107%)	299 (99%)	2 (1%)	84	61
2	C	2/2 (100%)	2 (100%)	0	100	100
2	E	2/2 (100%)	2 (100%)	0	100	100
2	G	2/2 (100%)	2 (100%)	0	100	100
2	I	2/2 (100%)	2 (100%)	0	100	100
All	All	1196/1132 (106%)	1193 (100%)	3 (0%)	92	78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	ASP
1	F	110	GLN
1	F	185	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	110	GLN
1	F	115	GLN
1	B	115	GLN
1	B	246	GLN
1	B	269	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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$
2	PSA	E	6	2	14,14,15	1.46	1 (7%)	15,17,19	1.80	4 (26%)
2	PSA	I	4	2	14,14,15	1.15	1 (7%)	15,17,19	1.70	2 (13%)
2	PSA	I	6	2	11,12,15	0.80	0	10,15,19	0.77	0
2	PSA	C	6	2	11,12,15	1.12	1 (9%)	10,15,19	1.61	2 (20%)
2	PSA	G	6[A]	2	11,12,15	0.36	0	10,15,19	0.88	1 (10%)
2	PSA	G	6[B]	2	11,12,15	0.43	0	10,15,19	0.41	0
2	PSA	G	4	2	14,14,15	0.94	1 (7%)	15,17,19	1.09	1 (6%)
2	PSA	E	4	2	14,14,15	0.97	1 (7%)	15,17,19	1.34	2 (13%)
2	PSA	C	4	2	14,14,15	1.01	1 (7%)	15,17,19	1.70	2 (13%)

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
2	PSA	E	6	2	-	0/11/11/12	0/1/1/1
2	PSA	I	4	2	-	5/11/11/12	0/1/1/1
2	PSA	I	6	2	-	0/8/8/12	0/1/1/1
2	PSA	C	6	2	-	0/8/8/12	0/1/1/1
2	PSA	G	6[A]	2	-	0/8/8/12	0/1/1/1
2	PSA	G	6[B]	2	-	0/8/8/12	0/1/1/1
2	PSA	G	4	2	-	5/11/11/12	0/1/1/1
2	PSA	E	4	2	-	5/11/11/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSA	C	4	2	-	3/11/11/12	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	6	PSA	O-C	4.60	1.46	1.19
2	I	4	PSA	O-C	3.54	1.40	1.19
2	C	6	PSA	CB-CA	3.00	1.58	1.53
2	C	4	PSA	O-C	2.69	1.35	1.19
2	G	4	PSA	O-C	2.44	1.33	1.19

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	PSA	O-C-CM	-5.19	110.30	125.43
2	E	6	PSA	O-C-CM	-4.85	111.29	125.43
2	C	4	PSA	O-C-CM	-4.84	111.31	125.43
2	G	4	PSA	O-C-CM	-3.40	115.51	125.43
2	C	6	PSA	CG-CB-CA	-3.10	106.88	113.46

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	PSA	OH-CH-CM-C
2	E	4	PSA	CA-CB-CG-CD2
2	E	4	PSA	CA-CB-CG-CD1
2	I	4	PSA	CA-CH-CM-C
2	I	4	PSA	OH-CH-CM-C

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	PSA	2	0

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

12 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	PEG	B	403	-	6,6,6	1.13	1 (16%)	5,5,5	1.13	0
3	PEG	D	401	-	6,6,6	0.56	0	5,5,5	1.37	1 (20%)
3	PEG	B	401	-	6,6,6	0.32	0	5,5,5	0.34	0
3	PEG	F	402	-	6,6,6	0.36	0	5,5,5	0.47	0
3	PEG	D	406	-	6,6,6	0.61	0	5,5,5	2.19	3 (60%)
3	PEG	F	403	-	6,6,6	0.52	0	5,5,5	0.41	0
3	PEG	B	402	-	6,6,6	0.51	0	5,5,5	0.53	0
3	PEG	D	405	-	6,6,6	0.46	0	5,5,5	0.24	0
3	PEG	D	403	-	6,6,6	0.39	0	5,5,5	0.38	0
3	PEG	F	401	-	6,6,6	0.45	0	5,5,5	0.28	0
3	PEG	D	404	-	6,6,6	0.54	0	5,5,5	0.77	0
3	PEG	D	402	-	6,6,6	0.51	0	5,5,5	1.42	1 (20%)

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	PEG	B	403	-	-	2/4/4/4	-
3	PEG	D	401	-	-	0/4/4/4	-
3	PEG	B	401	-	-	0/4/4/4	-
3	PEG	F	402	-	-	1/4/4/4	-
3	PEG	D	406	-	-	4/4/4/4	-
3	PEG	F	403	-	-	2/4/4/4	-
3	PEG	B	402	-	-	2/4/4/4	-
3	PEG	D	405	-	-	2/4/4/4	-
3	PEG	D	403	-	-	2/4/4/4	-
3	PEG	F	401	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	D	404	-	-	3/4/4/4	-
3	PEG	D	402	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	PEG	O2-C2	2.02	1.50	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	406	PEG	C3-O2-C2	3.67	129.20	113.29
3	D	402	PEG	C3-O2-C2	2.58	124.47	113.29
3	D	406	PEG	O2-C2-C1	2.31	120.20	110.07
3	D	406	PEG	O2-C3-C4	2.10	119.31	110.07
3	D	401	PEG	O1-C1-C2	-2.03	100.06	111.81

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	406	PEG	C1-C2-O2-C3
3	B	403	PEG	O1-C1-C2-O2
3	B	403	PEG	O2-C3-C4-O4
3	D	404	PEG	C1-C2-O2-C3
3	D	402	PEG	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	PEG	1	7
3	D	401	PEG	1	7
3	D	406	PEG	2	0
3	D	403	PEG	1	0
3	D	402	PEG	12	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	339/339 (100%)	0.06	13 (3%) 40 37	8, 13, 24, 38	3 (0%)
1	B	339/339 (100%)	0.01	12 (3%) 44 41	7, 12, 24, 35	4 (1%)
1	D	339/339 (100%)	-0.23	3 (0%) 84 85	6, 9, 18, 29	1 (0%)
1	F	339/339 (100%)	-0.13	10 (2%) 51 49	6, 11, 21, 33	1 (0%)
2	C	3/7 (42%)	0.13	0 100 100	11, 11, 12, 14	0
2	E	4/7 (57%)	1.32	1 (25%) 0 0	8, 9, 9, 31	0
2	G	3/7 (42%)	-0.43	0 100 100	11, 11, 11, 11	0
2	I	3/7 (42%)	0.47	0 100 100	15, 15, 15, 19	0
All	All	1369/1384 (98%)	-0.06	39 (2%) 53 50	6, 11, 22, 38	9 (0%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ALA	6.1
2	E	7	ALA	6.1
1	F	252	TYR	5.2
1	B	252	TYR	4.9
1	A	252	TYR	4.7

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PSA	C	6	12/15	0.81	0.15	14,17,21,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PSA	I	6	12/15	0.85	0.17	18,22,31,33	0
2	PSA	E	6	14/15	0.90	0.11	10,11,26,30	0
2	PSA	I	4	14/15	0.94	0.07	11,14,17,17	0
2	PSA	G	6[A]	12/15	0.94	0.09	12,13,15,15	12
2	PSA	G	6[B]	12/15	0.94	0.09	12,13,18,18	12
2	PSA	G	4	14/15	0.97	0.07	8,9,13,14	0
2	PSA	C	4	14/15	0.97	0.06	8,11,14,15	0
2	PSA	E	4	14/15	0.98	0.06	6,7,9,9	0

### 6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	PEG	B	402	7/7	0.14	0.35	56,59,64,64	0
3	PEG	D	401	7/7	0.21	0.41	40,45,54,56	7
3	PEG	D	402	7/7	0.56	0.41	30,33,36,36	0
3	PEG	F	403	7/7	0.67	0.21	35,35,37,37	0
3	PEG	D	404	7/7	0.69	0.20	35,36,38,39	0
3	PEG	B	403	7/7	0.70	0.25	32,34,38,40	1
3	PEG	F	401	7/7	0.73	0.22	46,50,55,56	0
3	PEG	D	403	7/7	0.73	0.19	48,51,52,53	0
3	PEG	F	402	7/7	0.76	0.19	42,43,46,47	0
3	PEG	D	405	7/7	0.82	0.12	40,42,45,47	0
3	PEG	D	406	7/7	0.86	0.29	25,29,32,37	0
3	PEG	B	401	7/7	0.89	0.10	20,21,24,26	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.