



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2021 – 05:28 am BST

PDB ID : 7AGC
Title : Protease Sapp1p from *Candida parapsilosis* in complex with KB74
Authors : Dostal, J.; Heidingsfeld, O.; Brynda, J.
Deposited on : 2020-09-22
Resolution : 1.35 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 : 2.18
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

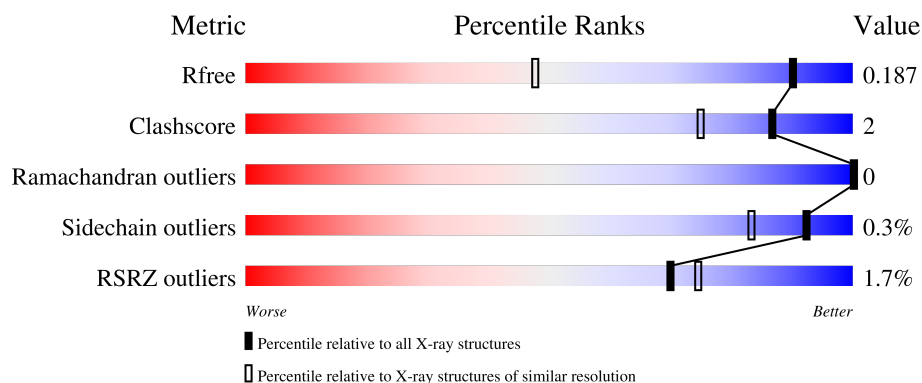
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	339	<div> <div>3%</div> <div>96%</div> <div>.</div> </div>
1	B	339	<div> <div>%</div> <div>98%</div> <div>.</div> </div>
1	D	339	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>
1	F	339	<div> <div>%</div> <div>96%</div> <div>.</div> </div>
2	C	7	<div> <div>57%</div> <div>14%</div> <div>29%</div> </div>

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11654 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
			2576	1608	419	545	4			
1	B	339	Total	C	N	O	S	3	22	0
			2630	1641	427	558	4			
1	D	339	Total	C	N	O	S	0	17	0
			2593	1617	418	554	4			
1	F	339	Total	C	N	O	S	0	17	0
			2594	1617	417	556	4			

- Molecule 2 is a protein called KB74.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			40	29	4	7			
2	I	5	Total	C	N	O	0	0	0
			40	29	4	7			
2	C	5	Total	C	N	O	0	0	0
			40	29	4	7			
2	G	5	Total	C	N	O	0	0	0
			40	29	4	7			

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



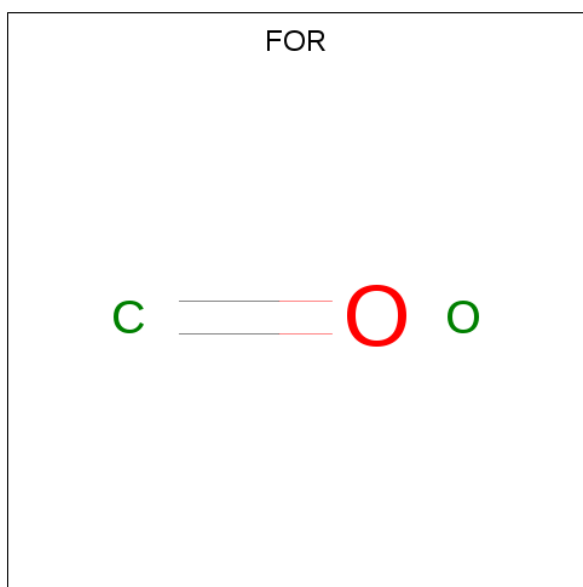
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



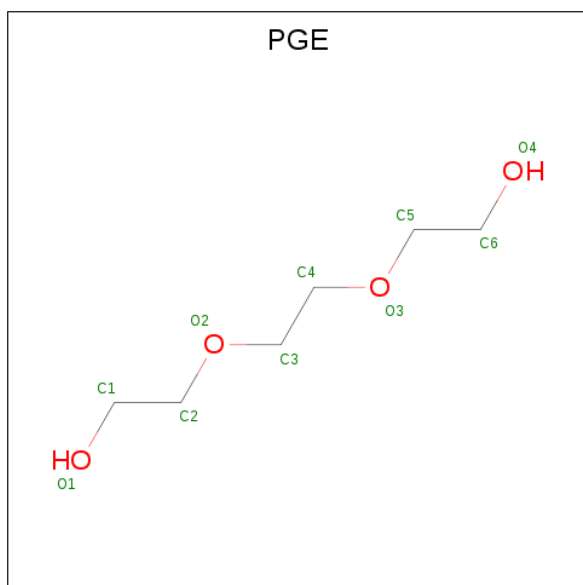
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is FORMYL GROUP (three-letter code: FOR) (formula: CH_2O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			2	1	1		
5	I	1	Total	C	O	0	0
			2	1	1		
5	C	1	Total	C	O	0	0
			2	1	1		
5	G	1	Total	C	O	0	0
			2	1	1		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			10	6	4		

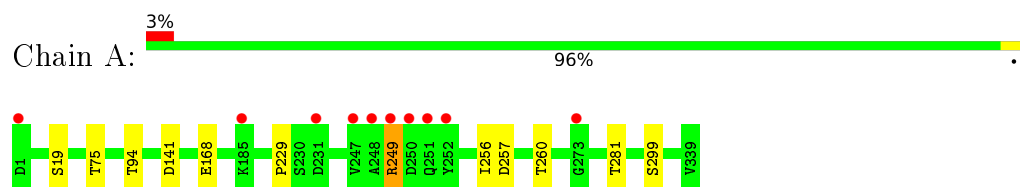
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	245	Total	O	0	1
			246	246		
7	B	296	Total	O	0	0
			296	296		
7	D	238	Total	O	0	1
			239	239		
7	E	3	Total	O	0	0
			3	3		
7	F	262	Total	O	0	0
			262	262		
7	I	3	Total	O	0	0
			3	3		
7	C	5	Total	O	0	0
			5	5		
7	G	3	Total	O	0	0
			3	3		

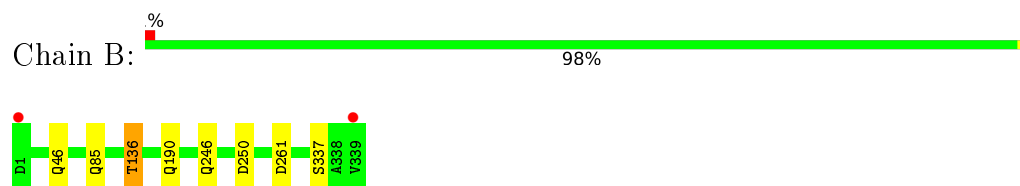
3 Residue-property plots [i](#)

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.

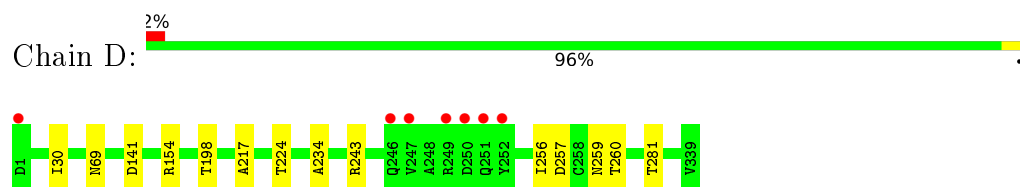
- Molecule 1: Candidapepsin



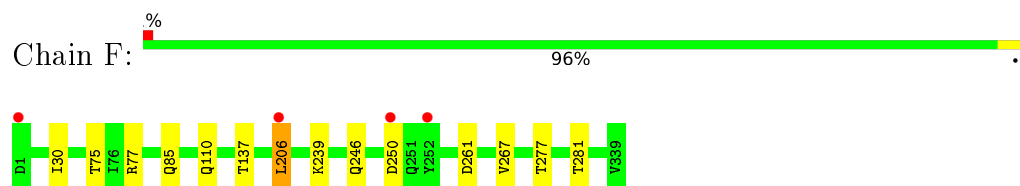
- Molecule 1: Candidapepsin



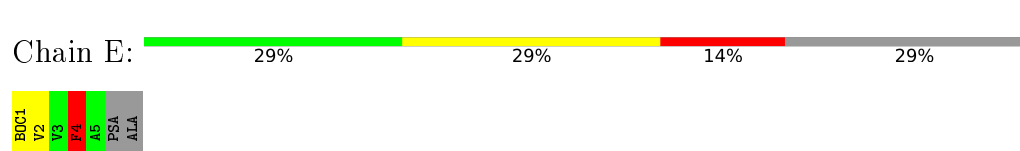
- Molecule 1: Candidapepsin



- Molecule 1: Candidapepsin



- Molecule 2: KB74



- Molecule 2: KB74

Chain I:  57% 14% 29%

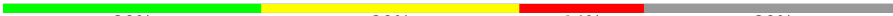


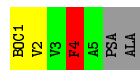
• Molecule 2: KB74

Chain C:  57% 14% 29%



• Molecule 2: KB74

Chain G:  29% 29% 14% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.25Å 87.36Å 157.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.84 – 1.35 48.61 – 1.35	Depositor EDS
% Data completeness (in resolution range)	96.3 (78.84-1.35) 96.3 (48.61-1.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.163 , 0.186 0.165 , 0.187	Depositor DCC
R_{free} test set	12767 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	8.9	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.054 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11654	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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 56.87 % 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 2.5688e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FOR, PEG, PGE, MES, 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	0.58	0/2653	0.78	2/3611 (0.1%)
1	B	0.63	2/2732 (0.1%)	0.78	3/3715 (0.1%)
1	D	0.60	0/2681	0.77	4/3649 (0.1%)
1	F	0.60	0/2685	0.76	3/3658 (0.1%)
2	C	1.21	0/17	0.68	0/21
2	E	0.79	0/17	0.77	0/21
2	G	0.67	0/17	0.79	0/21
2	I	0.77	0/17	0.74	0/21
All	All	0.61	2/10819 (0.0%)	0.77	12/14717 (0.1%)

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	2
2	G	0	2
2	I	0	2
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337[A]	SER	N-CA	-5.89	1.34	1.46
1	B	337[B]	SER	N-CA	-5.89	1.34	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	261	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	243	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	F	206	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	337[A]	SER	N-CA-CB	-5.55	102.17	110.50
1	B	337[B]	SER	N-CA-CB	-5.55	102.17	110.50
1	D	141	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	257	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	B	261	ASP	CB-CG-OD1	5.34	123.10	118.30
1	D	243	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	D	154	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	F	77	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	141	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	4	PSA	Mainchain,Peptide
2	E	4	PSA	Mainchain,Peptide
2	G	4	PSA	Mainchain,Peptide
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	2576	0	2511	10	0
1	B	2630	0	2571	5	0
1	D	2593	0	2519	10	0
1	F	2594	0	2514	14	0
2	C	40	0	44	0	0
2	E	40	0	43	5	0
2	G	40	0	43	4	0
2	I	40	0	44	0	0
3	A	12	0	13	0	0
4	A	7	0	10	0	0
4	B	7	0	10	0	0
5	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	2	0	0	0	0
5	G	2	0	0	0	0
5	I	2	0	0	0	0
6	I	10	0	14	0	0
7	A	246	0	0	2	0
7	B	296	0	0	3	0
7	C	5	0	0	0	0
7	D	239	0	0	3	0
7	E	3	0	0	0	0
7	F	262	0	0	5	0
7	G	3	0	0	0	0
7	I	3	0	0	0	0
All	All	11654	0	10336	42	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 2.

All (42) 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	1.59	1.20
1:B:136[A]:THR:OG1	7:B:501:HOH:O	1.63	1.15
1:F:137:THR:OG1	7:F:401:HOH:O	1.81	0.96
1:D:257[B]:ASP:CG	1:D:259[B]:ASN:OD1	2.16	0.83
1:D:234:ALA:N	7:D:403:HOH:O	2.20	0.74
1:A:249:ARG:HH11	1:A:249:ARG:HG3	1.52	0.73
2:G:1:BOC:C	2:G:2:VAL:CA	2.66	0.73
1:B:136[A]:THR:HG21	7:B:738:HOH:O	1.89	0.71
2:G:1:BOC:O2	2:G:2:VAL:N	2.25	0.69
1:D:257[B]:ASP:HB3	1:D:260[B]:THR:HG23	1.75	0.69
2:E:1:BOC:O2	2:E:2:VAL:N	2.27	0.66
1:D:256:ILE:HG12	1:D:260[B]:THR:HG21	1.81	0.63
1:F:277[B]:THR:HG23	7:F:477:HOH:O	1.99	0.62
1:A:19[B]:SER:OG	1:A:94:THR:HB	2.01	0.61
1:B:246:GLN:HE21	1:B:250:ASP:H	1.48	0.60
1:D:224:THR:HG1	2:E:2:VAL:N	2.01	0.58
1:B:190[B]:GLN:NE2	7:B:502:HOH:O	2.35	0.58
1:D:281[B]:THR:HG23	7:D:596:HOH:O	2.02	0.58
1:A:249:ARG:HH11	1:A:249:ARG:CG	2.17	0.57
1:F:277[B]:THR:HG21	7:F:466:HOH:O	2.04	0.56
1:A:75[A]:THR:HG21	1:B:85:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75[A]:THR:HG23	7:A:504:HOH:O	2.08	0.54
2:E:1:BOC:C	2:E:2:VAL:CA	2.84	0.53
1:D:30:ILE:HD13	2:E:4:PSA:HE1	1.91	0.52
2:E:1:BOC:O1	2:E:2:VAL:N	2.40	0.50
1:F:85:GLN:HB2	1:F:110:GLN:HG3	1.95	0.49
1:F:30:ILE:HD13	2:G:4:PSA:HE1	1.96	0.48
1:D:69[A]:ASN:ND2	7:D:401:HOH:O	0.72	0.48
1:D:198[B]:THR:HG23	1:D:217:ALA:N	2.28	0.47
1:A:281[A]:THR:HG23	7:A:702:HOH:O	2.14	0.47
1:F:30:ILE:HD13	2:G:4:PSA:CE1	2.47	0.45
1:A:249:ARG:CG	1:A:249:ARG:NH1	2.75	0.44
1:F:246:GLN:HE21	1:F:250:ASP:H	1.65	0.44
1:A:229:PRO:HA	1:A:299:SER:O	2.17	0.44
1:F:75[B]:THR:HG22	1:F:85:GLN:HG3	2.00	0.44
1:F:75[B]:THR:HG22	1:F:85:GLN:CG	2.48	0.44
1:A:256:ILE:HG12	1:A:260[B]:THR:HG21	2.01	0.43
1:F:281[A]:THR:HG23	7:F:515:HOH:O	2.18	0.42
1:F:206:LEU:CD2	1:F:239:LYS:CG	2.97	0.42
1:F:267:VAL:HG22	1:F:277[B]:THR:HG22	2.03	0.41
1:A:168:GLU:OE1	1:F:239:LYS:NZ	2.53	0.41
1:F:281[A]:THR:HG23	7:F:512:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/339 (103%)	342 (98%)	7 (2%)	0	100	100
1	B	358/339 (106%)	353 (99%)	5 (1%)	0	100	100
1	D	354/339 (104%)	348 (98%)	6 (2%)	0	100	100
1	F	354/339 (104%)	348 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	2/7 (29%)	1 (50%)	1 (50%)	0	100	100
2	E	2/7 (29%)	2 (100%)	0	0	100	100
2	G	2/7 (29%)	1 (50%)	1 (50%)	0	100	100
2	I	2/7 (29%)	2 (100%)	0	0	100	100
All	All	1423/1384 (103%)	1397 (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%)	292 (100%)	1 (0%)	92	83
1	B	302/281 (108%)	298 (99%)	4 (1%)	69	37
1	D	296/281 (105%)	296 (100%)	0	100	100
1	F	297/281 (106%)	297 (100%)	0	100	100
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%)	1191 (100%)	5 (0%)	92	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	ARG
1	B	46[A]	GLN
1	B	46[B]	GLN
1	B	136[A]	THR
1	B	136[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	115	GLN
1	A	286	GLN
1	B	115	GLN
1	B	246	GLN
1	B	269	ASN
1	D	115	GLN
1	F	110	GLN
1	F	115	GLN
1	F	205	ASN
1	F	246	GLN

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
2	PSA	E	4	2	14,14,15	1.17	1 (7%)	15,17,19	1.51	2 (13%)
2	PSA	C	4	2	14,14,15	1.00	1 (7%)	15,17,19	1.24	1 (6%)
2	PSA	G	4	2	14,14,15	0.91	0	15,17,19	1.18	2 (13%)
2	PSA	I	4	2	14,14,15	1.21	2 (14%)	15,17,19	1.30	1 (6%)

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	4	2	-	5/11/11/12	0/1/1/1
2	PSA	C	4	2	-	5/11/11/12	0/1/1/1
2	PSA	G	4	2	-	2/11/11/12	0/1/1/1
2	PSA	I	4	2	-	5/11/11/12	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	PSA	CH-CA	-2.96	1.50	1.53
2	I	4	PSA	CM-C	2.46	1.56	1.49
2	I	4	PSA	CH-CA	-2.37	1.50	1.53
2	C	4	PSA	CH-CA	-2.20	1.51	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	PSA	O-C-CM	-3.73	114.56	125.43
2	E	4	PSA	O-C-CM	-3.66	114.77	125.43
2	C	4	PSA	O-C-CM	-3.27	115.90	125.43
2	G	4	PSA	O-C-CM	-2.99	116.73	125.43
2	E	4	PSA	CG-CB-CA	2.61	119.00	113.46
2	G	4	PSA	CG-CB-CA	2.29	118.31	113.46

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	E	4	PSA	OH-CH-CM-C
2	C	4	PSA	OH-CH-CM-C
2	G	4	PSA	OH-CH-CM-C

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	PSA	1	0
2	G	4	PSA	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
5	FOR	I	101	2	0,1,1	0.00	-	-		
5	FOR	G	101	2	0,1,1	0.00	-	-		
5	FOR	E	101	2	0,1,1	0.00	-	-		
5	FOR	C	101	2	0,1,1	0.00	-	-		
4	PEG	A	402	-	6,6,6	0.42	0	5,5,5	0.27	0
3	MES	A	401	-	12,12,12	2.19	1 (8%)	14,16,16	1.66	3 (21%)
4	PEG	B	401	-	6,6,6	0.49	0	5,5,5	0.37	0
6	PGE	I	102	-	9,9,9	0.53	0	8,8,8	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	402	-	-	2/4/4/4	-
4	PEG	B	401	-	-	0/4/4/4	-
3	MES	A	401	-	-	2/6/14/14	0/1/1/1
6	PGE	I	102	-	-	2/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	MES	C8-S	-7.21	1.67	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	MES	O1S-S-C8	3.39	111.00	106.92
3	A	401	MES	O2S-S-C8	3.37	110.97	106.92
3	A	401	MES	O3S-S-C8	2.02	109.03	105.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	102	PGE	C4-C3-O2-C2
4	A	402	PEG	O2-C3-C4-O4
3	A	401	MES	C8-C7-N4-C5
4	A	402	PEG	C4-C3-O2-C2
6	I	102	PGE	O1-C1-C2-O2
3	A	401	MES	C8-C7-N4-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1
2	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	1:BOC	C	2:VAL	N	1.97
1	G	1:BOC	C	2:VAL	N	1.75

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	339/339 (100%)	0.02	10 (2%) 51 59	6, 11, 20, 39	3 (0%)
1	B	339/339 (100%)	-0.07	2 (0%) 89 91	5, 9, 16, 26	3 (0%)
1	D	339/339 (100%)	0.09	7 (2%) 63 69	7, 10, 22, 54	0
1	F	339/339 (100%)	0.01	4 (1%) 79 83	6, 10, 19, 30	0
2	C	3/7 (42%)	-0.04	0 100 100	8, 8, 8, 10	0
2	E	3/7 (42%)	0.40	0 100 100	12, 12, 12, 14	0
2	G	3/7 (42%)	-0.14	0 100 100	8, 8, 10, 10	0
2	I	3/7 (42%)	-0.25	0 100 100	9, 9, 10, 10	0
All	All	1368/1384 (98%)	0.01	23 (1%) 70 74	5, 10, 19, 54	6 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	250[A]	ASP	4.8
1	D	252	TYR	4.8
1	D	249	ARG	4.4
1	A	250	ASP	3.9
1	A	252	TYR	3.5
1	D	1	ASP	3.1
1	A	185	LYS	3.0
1	D	246	GLN	3.0
1	F	252	TYR	2.8
1	D	251	GLN	2.7
1	A	273	GLY	2.7
1	B	339[A]	VAL	2.6
1	A	1	ASP	2.6
1	A	247	VAL	2.4
1	A	249	ARG	2.4
1	A	248	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1	ASP	2.3
1	A	251	GLN	2.2
1	F	1	ASP	2.2
1	D	247	VAL	2.1
1	F	250	ASP	2.1
1	F	206	LEU	2.1
1	A	231	ASP	2.0

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, 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
2	PSA	E	4	14/15	0.95	0.08	8,11,15,15	0
2	PSA	I	4	14/15	0.96	0.08	7,8,10,11	0
2	PSA	G	4	14/15	0.96	0.07	7,8,11,11	0
2	PSA	C	4	14/15	0.97	0.07	6,7,8,8	0

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
4	PEG	A	402	7/7	0.74	0.15	25,29,30,33	0
6	PGE	I	102	10/10	0.80	0.19	20,22,27,28	0
4	PEG	B	401	7/7	0.81	0.14	25,26,26,27	0
3	MES	A	401	12/12	0.86	0.34	18,26,31,31	1
5	FOR	C	101	2/2	0.92	0.15	12,12,12,14	0
5	FOR	E	101	2/2	0.92	0.26	17,17,17,18	0
5	FOR	G	101	2/2	0.95	0.14	15,15,15,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	FOR	I	101	2/2	0.96	0.07	12,12,12,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.