Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 11:07 PM EDT

PDB ID	:	5LAK
Title	:	Ligand-bound structure of Cavally Virus 3CL Protease
Authors	:	Kanitz, M.; Heine, A.; Diederich, W.E.
Deposited on	:	2016-06-14
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

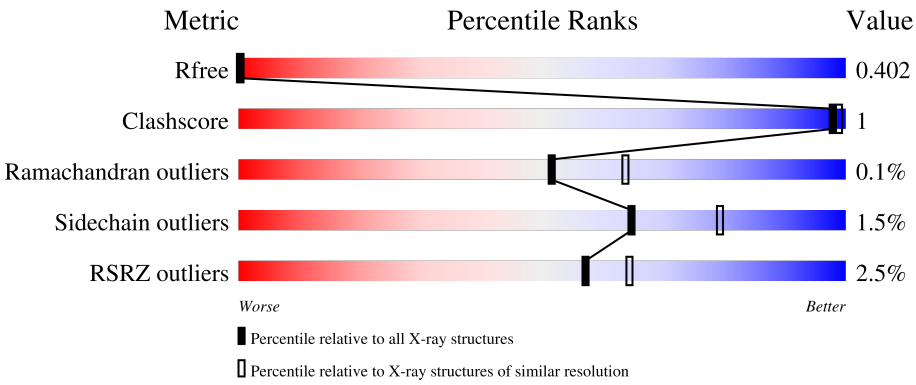
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	314	% 93%
1	B	314	3% 92% 6%
1	C	314	2% 94%
1	D	314	4% 89% 9%
2	I	5	80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	5	80% 20%
2	K	5	80% 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17521 atoms, of which 8197 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.

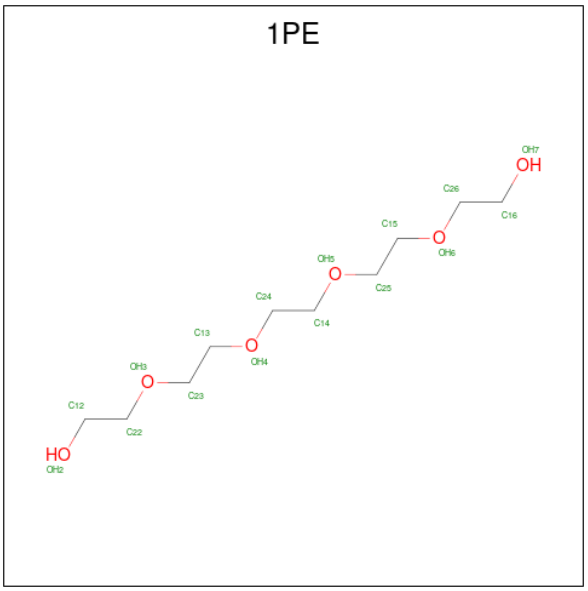
- Molecule 1 is a protein called 3Cl Protease.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	303	4518	1486	2188	392	438	14	0	2	0
1	B	294	4211	1396	2010	375	417	13	0	0	0
1	C	303	4296	1437	2034	379	433	13	0	0	0
1	D	286	4089	1368	1942	360	406	13	0	0	0

- Molecule 2 is a protein called BEZ-TYR-TYR-ASN-ECC Peptide inhibitor.

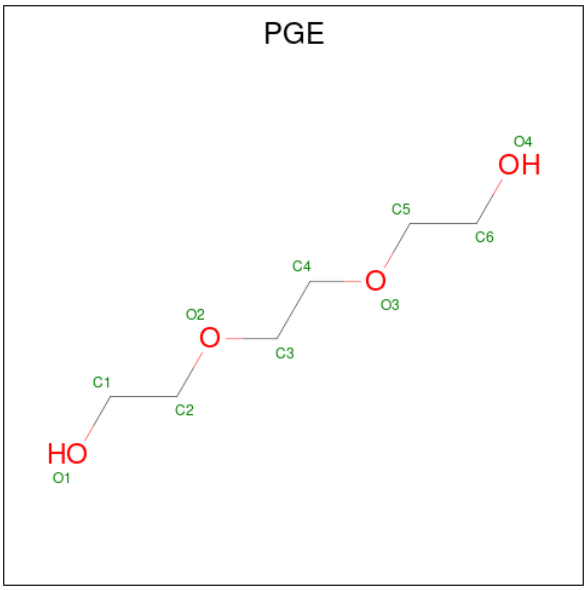
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	5	49	34	6	9	0	0	0
2	J	5	49	34	6	9	0	0	0
2	K	5	48	34	6	8	0	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	16	10	6	0	0
			Total	C	O		
3	C	1	12	8	4	0	0
			Total	C	O		
3	D	1	13	8	5	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	B	1	24	6	14	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	C	1	17	5	9	3	0	0

- Molecule 5 is water.

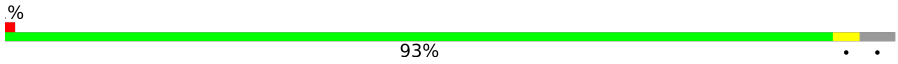
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	67	67	67	0	0
			Total	O		
5	B	32	32	32	0	0
			Total	O		
5	C	48	48	48	0	0
			Total	O		
5	D	32	32	32	0	0

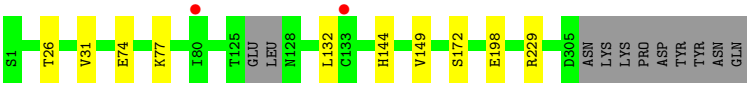
3 Residue-property plots (i)

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: 3Cl Protease

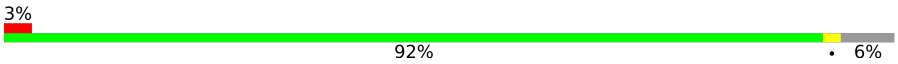
Chain A:

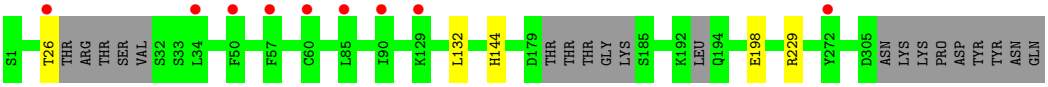




- Molecule 1: 3Cl Protease

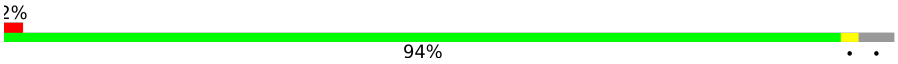
Chain B:

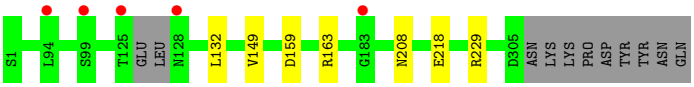




- Molecule 1: 3Cl Protease

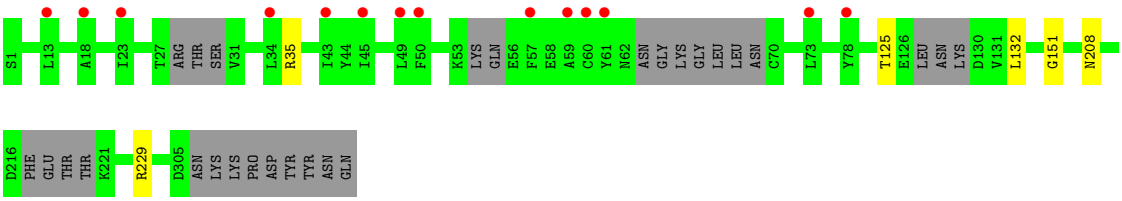
Chain C:





- Molecule 1: 3Cl Protease

Chain D:



- Molecule 2: BEZ-TYR-TYR-ASN-ECC Peptide inhibitor

Chain I:

• Molecule 2: BEZ-TYR-TYR-ASN-ECC Peptide inhibitor

Chain J:

• Molecule 2: BEZ-TYR-TYR-ASN-ECC Peptide inhibitor

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.19Å 110.15Å 98.50Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	45.33 – 2.30 47.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.33-2.30) 99.3 (47.61-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.208 , 0.230 0.399 , 0.402	Depositor DCC
R_{free} test set	3274 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17521	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BEZ, ECC, 1PE, PGE

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	0.26	0/2394	0.49	0/3264
1	B	0.24	0/2251	0.45	0/3073
1	C	0.25	0/2317	0.46	0/3173
1	D	0.25	0/2196	0.48	0/3002
2	I	0.48	0/33	0.56	0/44
2	J	0.48	0/33	0.31	0/44
2	K	0.50	0/32	0.87	0/42
All	All	0.25	0/9256	0.47	0/12642

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	I	1	0
2	K	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	2	TYR	CA
2	K	2	TYR	CA

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	2330	2188	2195	4	0
1	B	2201	2010	2023	1	0
1	C	2262	2034	2046	4	0
1	D	2147	1942	1958	2	0
2	I	49	0	38	1	0
2	J	49	0	38	1	0
2	K	48	0	37	0	0
3	A	16	0	22	0	0
3	C	12	0	14	3	0
3	D	13	0	17	1	0
4	B	10	14	14	0	0
4	C	8	9	9	0	0
5	A	67	0	0	0	0
5	B	32	0	0	0	0
5	C	48	0	0	0	0
5	D	32	0	0	0	0
All	All	9324	8197	8411	12	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 1.

All (12) 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:C:159:ASP:OD2	1:C:163:ARG:NH1	2.20	0.74
1:C:208:ASN:HD21	3:C:402:1PE:H131	1.58	0.69
1:C:208:ASN:HD21	3:C:402:1PE:H221	1.66	0.61
1:D:208:ASN:HD21	3:D:401:1PE:H231	1.71	0.56
1:A:172:SER:HB3	2:I:2:TYR:H	1.77	0.50
1:A:74:GLU:OE1	1:A:77:LYS:NZ	2.46	0.48
1:C:218:GLU:O	2:J:2:TYR:OH	2.33	0.44
1:D:35:ARG:NH2	1:D:151:GLY:O	2.48	0.43
1:A:26:THR:HG23	1:A:31:VAL:HG22	2.00	0.43
3:C:402:1PE:H131	3:C:402:1PE:H221	1.76	0.42
1:A:144:HIS:CE1	1:A:198:GLU:HB3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:HIS:CE1	1:B:198:GLU:HB3	2.55	0.41

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	301/314 (96%)	299 (99%)	2 (1%)	0	100	100
1	B	286/314 (91%)	284 (99%)	2 (1%)	0	100	100
1	C	299/314 (95%)	295 (99%)	4 (1%)	0	100	100
1	D	274/314 (87%)	270 (98%)	4 (2%)	0	100	100
2	I	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
2	J	3/5 (60%)	3 (100%)	0	0	100	100
2	K	3/5 (60%)	2 (67%)	0	1 (33%)	0	0
All	All	1169/1271 (92%)	1155 (99%)	13 (1%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	2	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	247/284 (87%)	244 (99%)	3 (1%)	71 84
1	B	226/284 (80%)	223 (99%)	3 (1%)	69 82
1	C	229/284 (81%)	226 (99%)	3 (1%)	69 82
1	D	218/284 (77%)	215 (99%)	3 (1%)	67 81
2	I	3/3 (100%)	2 (67%)	1 (33%)	0 0
2	J	3/3 (100%)	3 (100%)	0	100 100
2	K	3/3 (100%)	2 (67%)	1 (33%)	0 0
All	All	929/1145 (81%)	915 (98%)	14 (2%)	65 79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	149	VAL
1	A	229	ARG
1	B	26	THR
1	B	132	LEU
1	B	229	ARG
1	C	132	LEU
1	C	149	VAL
1	C	229	ARG
1	D	125	THR
1	D	132	LEU
1	D	229	ARG
2	I	2	TYR
2	K	2	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	208	ASN
1	D	208	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)

3 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	ECC	K	5	2,1	8,8,8	0.10	0	8,9,9	0.38	0
2	ECC	I	5	2,1	8,8,8	0.14	0	8,9,9	0.24	0
2	ECC	J	5	2,1	8,8,8	0.12	0	8,9,9	0.40	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
2	ECC	K	5	2,1	-	0/7/7/7	-
2	ECC	I	5	2,1	-	1/7/7/7	-
2	ECC	J	5	2,1	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	5	ECC	O-C-CA-N
2	J	5	ECC	O-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	1PE	C	402	-	11,11,15	0.17	0	10,10,14	0.10	0
3	1PE	A	401	-	15,15,15	0.15	0	14,14,14	0.18	0
4	PGE	C	401	-	7,7,9	0.30	0	6,6,8	0.27	0
3	1PE	D	401	-	12,12,15	0.14	0	11,11,14	0.15	0
4	PGE	B	401	-	9,9,9	0.32	0	8,8,8	0.54	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	1PE	C	402	-	-	6/9/9/13	-
3	1PE	A	401	-	-	0/13/13/13	-
4	PGE	C	401	-	-	3/5/5/7	-
3	1PE	D	401	-	-	4/10/10/13	-
4	PGE	B	401	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	1PE	OH4-C13-C23-OH3
4	B	401	PGE	O2-C3-C4-O3
4	C	401	PGE	O2-C3-C4-O3
3	C	402	1PE	C13-C23-OH3-C22
3	D	401	1PE	C13-C23-OH3-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	402	1PE	C12-C22-OH3-C23
4	C	401	PGE	C4-C3-O2-C2
3	C	402	1PE	C23-C13-OH4-C24
3	D	401	1PE	OH5-C14-C24-OH4
4	B	401	PGE	C3-C4-O3-C5
4	B	401	PGE	O3-C5-C6-O4
4	C	401	PGE	O1-C1-C2-O2
4	B	401	PGE	C6-C5-O3-C4
3	D	401	1PE	C12-C22-OH3-C23
3	C	402	1PE	C24-C14-OH5-C25
3	C	402	1PE	C14-C24-OH4-C13
3	C	402	1PE	OH4-C13-C23-OH3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	1PE	3	0
3	D	401	1PE	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	303/314 (96%)	0.39	2 (0%)	87	91	25, 35, 50, 62	0
1	B	294/314 (93%)	0.58	9 (3%)	49	56	26, 49, 70, 82	0
1	C	303/314 (96%)	0.35	5 (1%)	70	76	29, 44, 61, 69	0
1	D	286/314 (91%)	0.50	14 (4%)	29	36	31, 46, 74, 84	0
2	I	3/5 (60%)	0.70	0	100	100	36, 36, 39, 44	0
2	J	3/5 (60%)	1.16	0	100	100	41, 41, 47, 58	0
2	K	3/5 (60%)	0.86	0	100	100	48, 48, 52, 56	0
All	All	1195/1271 (94%)	0.46	30 (2%)	57	64	25, 43, 68, 84	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	59	ALA	6.0
1	D	50	PHE	4.0
1	D	60	CYS	3.9
1	B	60	CYS	3.9
1	C	94	LEU	3.4
1	C	183	GLY	3.0
1	D	73	LEU	3.0
1	C	99	SER	2.8
1	B	129	LYS	2.8
1	D	49	LEU	2.7
1	B	90	ILE	2.6
1	B	34	LEU	2.6
1	B	57	PHE	2.6
1	B	85	LEU	2.5
1	C	128	ASN	2.5
1	D	57	PHE	2.5
1	D	13	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	26	THR	2.4
1	B	272	TYR	2.4
1	D	43	ILE	2.3
1	D	23	ILE	2.2
1	D	34	LEU	2.2
1	C	125	THR	2.2
1	D	78	TYR	2.1
1	B	50	PHE	2.0
1	A	80	ILE	2.0
1	D	45	ILE	2.0
1	D	61	TYR	2.0
1	A	133	CYS	2.0
1	D	18	ALA	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	ECC	K	5	9/9	0.93	0.19	40,43,48,50	0
2	ECC	J	5	9/9	0.96	0.16	35,38,43,48	0
2	ECC	I	5	9/9	0.97	0.15	25,30,32,34	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
3	1PE	D	401	13/16	0.84	0.17	38,44,50,51	0
4	PGE	B	401	10/10	0.86	0.27	38,62,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PGE	C	401	8/10	0.86	0.15	35,52,66,66	0
3	1PE	C	402	12/16	0.92	0.15	29,41,50,51	0
3	1PE	A	401	16/16	0.92	0.17	23,35,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.