

Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2023 – 08:47 PM EDT

PDB ID : 4WMD

Title: Crystal structure of catalytically inactive MERS-CoV 3CL protease (C148A)

in spacegroup C2221

Authors: Lountos, G.T.; Needle, D.; Waugh, D.S.

Deposited on : 2014-10-08

Resolution : 2.58 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 (1)) were used in the production of this report:

Mol Probity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

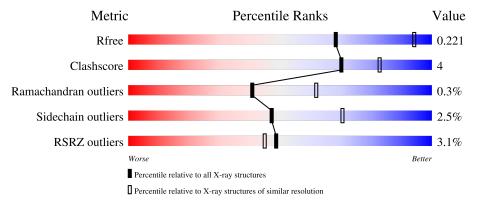
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	306	87%	11%	-
1	В	306	8%	11%	
1	С	306	91%	8%	•



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7289 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.

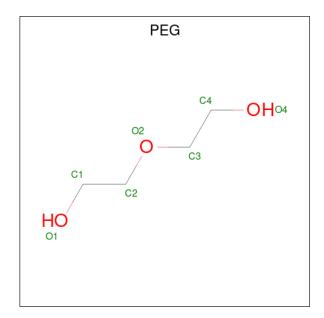
• Molecule 1 is a protein called ORF1a.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	301	Total	С	N	Ο	S	0	0	0
1	A	301	2293	1457	380	432	24	0	U	
1	В	304	Total	С	N	О	S	0	1	0
1	Б	304	2319	1473	385	437	24	0	1	
1	С	303	Total	С	N	О	S	0	9	0
1		303	2323	1474	388	437	24	0	<u> </u>	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ALA	CYS	engineered mutation	UNP W6A941
В	148	ALA	CYS	engineered mutation	UNP W6A941
С	148	ALA	CYS	engineered mutation	UNP W6A941

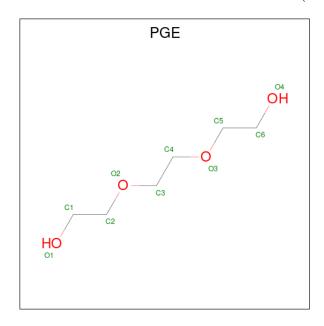
• Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 4 3	0	0
2	В	1	Total C O 7 4 3	0	0
2	С	1	Total C O 7 4 3	0	0

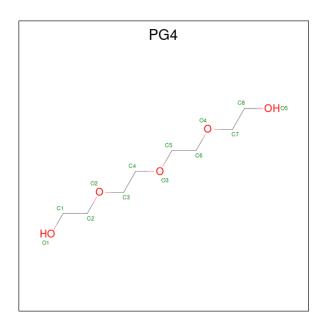
 \bullet Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $\mathrm{C_6H_{14}O_4}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	С	1	Total C O 10 6 4	0	0

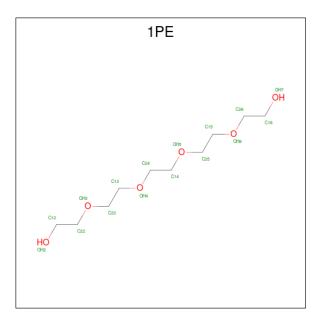
• Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).





Mol	Chain	Residues	Ato	ms		ZeroOcc	AltConf
4	В	1	Total 13	C 8	O 5	0	0

 \bullet Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $\mathrm{C_{10}H_{22}O_6}).$



Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
5	С	1	Total 16	C 10	O 6	0	0

• Molecule 6 is water.

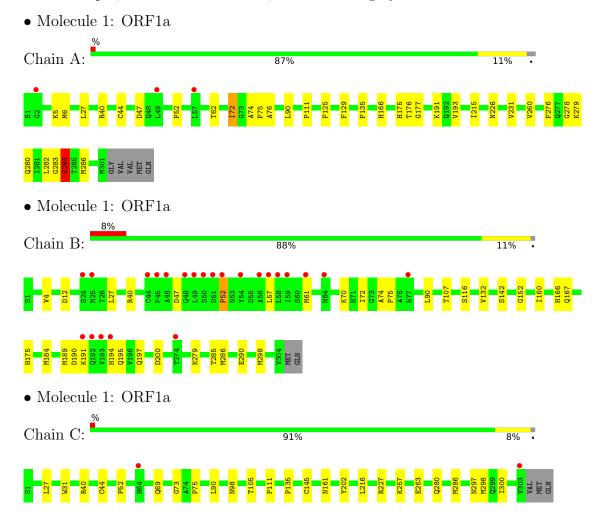


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	84	Total O 84 84	0	0
6	В	102	Total O 102 102	0	0
6	С	98	Total O 98 98	0	0



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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	81.02Å 168.52Å 250.52Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.16 - 2.58	Depositor
Resolution (A)	47.54 - 2.59	EDS
% Data completeness	99.4 (46.16-2.58)	Depositor
(in resolution range)	93.2 (47.54-2.59)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	2.49 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1448)	Depositor
D D	0.176 , 0.217	Depositor
R, R_{free}	0.180 , 0.221	DCC
R_{free} test set	2000 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 34.4	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7289	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: PG4, 1PE, PGE, PEG

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	\mathbf{angles}
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.46	0/2347	0.60	0/3195
1	В	0.45	0/2373	0.55	0/3231
1	С	0.45	0/2377	0.54	0/3236
All	All	0.45	0/7097	0.56	0/9662

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	LEU	Peptide

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	2293	0	2241	17	0
1	В	2319	0	2267	22	0
1	С	2323	0	2271	11	0
2	A	7	0	10	0	0
2	В	7	0	10	1	0
2	С	7	0	10	1	0
3	A	10	0	14	2	0
3	С	10	0	14	1	0
4	В	13	0	18	1	0
5	С	16	0	22	1	0
6	A	84	0	0	2	0
6	В	102	0	0	2	0
6	С	98	0	0	0	0
All	All	7289	0	6877	50	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 4.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance } (\text{\AA}) \end{array}$	Clash overlap (Å)
1:B:52:PRO:HD3	1:B:191:LYS:HG3	1.70	0.74
1:C:145:CYS:HA	3:C:403:PGE:H22	1.78	0.66
1:B:40:ARG:HA	1:B:90:LEU:HG	1.84	0.60
1:C:216:LEU:HD13	1:C:300:ILE:HG21	1.86	0.58
1:A:276:PHE:O	1:A:279:LYS:HB2	2.05	0.57
1:B:279:LYS:NZ	6:B:568:HOH:O	2.39	0.56
1:B:70:LYS:NZ	1:B:72:ILE:O	2.38	0.54
1:B:194:HIS:HD2	1:B:195:GLN:H	1.56	0.54
1:C:105:THR:OG1	1:C:161[B]:ASN:ND2	2.32	0.52
3:A:402:PGE:H12	6:A:568:HOH:O	2.09	0.52
1:A:40:ARG:HA	1:A:90:LEU:HG	1.92	0.52
1:C:216:LEU:HD21	1:C:257:LYS:HG3	1.93	0.51
1:B:200:ASP:HB3	2:B:401:PEG:H22	1.93	0.51
1:B:194:HIS:CD2	1:B:195:GLN:N	2.80	0.50
1:A:283:GLY:HA2	1:A:284:SER:CB	2.40	0.50
1:A:111:PRO:HB3	1:A:135:PRO:HA	1.93	0.50
1:B:166:HIS:HE1	1:B:175:HIS:HB3	1.77	0.49
1:A:191:LYS:HG3	1:A:193:VAL:HG12	1.94	0.49
1:B:189:MET:N	1:B:195:GLN:OE1	2.23	0.48
1:A:280:GLN:HB3	1:A:283:GLY:HA3	1.95	0.48
3:A:402:PGE:H42	6:A:568:HOH:O	2.12	0.48



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A		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:57:LEU:O	1:B:61:MET:HG2	2.13	0.48	
5:C:401:1PE:H242	5:C:401:1PE:H252	1.53	0.48	
1:A:278:GLY:HA3	1:A:279:LYS:HG2	1.94	0.48	
1:C:111:PRO:HB3	1:C:135:PRO:HA	1.95	0.48	
1:A:283:GLY:HA2	1:A:284:SER:HB3	1.96	0.47	
1:A:72:ILE:HG12	1:A:125:PRO:HD2	1.97	0.47	
1:B:70:LYS:NZ	6:B:536:HOH:O	2.46	0.47	
1:B:190:ASP:OD1	1:B:190:ASP:N	2.46	0.46	
1:A:129:PHE:CG	1:B:4:VAL:HG21	2.52	0.45	
1:C:227:ARG:HB3	1:C:263:GLU:HB3	1.98	0.45	
1:B:74:ALA:HA	1:B:75:PRO:HD3	1.84	0.45	
1:C:202:TYR:CE2	2:C:402:PEG:H22	2.51	0.45	
1:A:166:HIS:HE1	1:A:175:HIS:HB3	1.81	0.45	
1:B:189:MET:HE2	1:B:195:GLN:HG2	1.99	0.44	
1:B:12:ASP:HB3	1:B:160:ILE:HD11	1.99	0.44	
1:C:40:ARG:HA	1:C:90:LEU:HG	2.00	0.44	
1:A:176:THR:OG1	1:A:177:GLY:N	2.51	0.43	
1:A:74:ALA:HA	1:A:75:PRO:HD3	1.93	0.43	
1:A:286:MET:HG3	1:B:285:THR:HG21	2.00	0.43	
1:A:215:ILE:HD13	1:A:260:VAL:HG21	2.01	0.42	
1:A:6:MET:HE1	1:B:142:SER:HB3	2.01	0.42	
1:C:73:GLY:O	1:C:75:PRO:HD3	2.20	0.42	
1:B:132:VAL:HG21	1:B:290:GLU:HA	2.00	0.42	
1:B:116:SER:O	1:B:152:GLY:HA2	2.19	0.42	
1:C:31:TRP:CE2	1:C:98:ASN:HB2	2.55	0.42	
1:B:298:MET:CG	4:B:402:PG4:H32	2.50	0.41	
1:C:44:CYS:SG	1:C:52:PRO:HB3	2.61	0.41	
1:B:167:GLN:HG3	1:B:184:MET:SD	2.61	0.40	
1:A:44:CYS:SG	1:A:52:PRO:HB3	2.62	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	Perce	entiles
1	A	299/306~(98%)	283 (95%)	14 (5%)	2 (1%)	22	41
1	В	303/306 (99%)	290 (96%)	12 (4%)	1 (0%)	41	62
1	С	303/306 (99%)	298 (98%)	5 (2%)	0	100	100
All	All	905/918 (99%)	871 (96%)	31 (3%)	3 (0%)	41	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ALA
1	A	284	SER
1	В	52	PRO

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	252/256~(98%)	244 (97%)	8 (3%)	39	63	
1	В	255/256 (100%)	250 (98%)	5 (2%)	55	76	
1	С	255/256 (100%)	249 (98%)	6 (2%)	49	72	
All	All	762/768 (99%)	743 (98%)	19 (2%)	47	70	

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	27	LEU
1	A	47	ASP
1	A	62	THR
1	A	72	ILE
1	A	226	ASN
1	A	231	VAL
1	A	284	SER
1	В	27	LEU
1	В	47	ASP



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Mol	Chain	Res	Type
1	В	107	THR
1	В	197	GLN
1	В	286	MET
1	С	27	LEU
1	С	69	GLN
1	С	280	GLN
1	С	286	MET
1	С	297	ASN
1	С	298	MET

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

Mol	Chain	Res	Type
1	A	41	HIS
1	В	194	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	ol Type Chain Res		Link	Bond lengths			Bond angles			
MIOI	Iol Type Chain	Chain	nes	LILIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PGE	A	402	-	9,9,9	1.06	0	8,8,8	0.79	0
2	PEG	В	401	-	6,6,6	0.61	0	5,5,5	0.45	0
2	PEG	A	401	-	6,6,6	0.66	0	5,5,5	0.36	0
2	PEG	С	402	-	6,6,6	0.64	0	5,5,5	0.42	0
5	1PE	С	401	-	15,15,15	0.78	0	14,14,14	0.49	0
3	PGE	С	403	-	9,9,9	1.02	0	8,8,8	0.50	0
4	PG4	В	402	-	12,12,12	0.99	0	11,11,11	0.56	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	PGE	A	402	-	-	4/7/7/7	-
2	PEG	В	401	-	-	3/4/4/4	-
2	PEG	A	401	-	-	3/4/4/4	-
2	PEG	С	402	-	-	3/4/4/4	-
5	1PE	С	401	-	-	8/13/13/13	-
3	PGE	С	403	-	-	3/7/7/7	-
4	PG4	В	402	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	С	401	1PE	C24-C14-OH5-C25
3	A	402	PGE	O1-C1-C2-O2
3	A	402	PGE	O2-C3-C4-O3
5	С	401	1PE	OH4-C13-C23-OH3
5	С	401	1PE	OH5-C14-C24-OH4
3	С	403	PGE	O2-C3-C4-O3
4	В	402	PG4	O2-C3-C4-O3
2	В	401	PEG	C4-C3-O2-C2
2	A	401	PEG	O2-C3-C4-O4
3	С	403	PGE	O1-C1-C2-O2
5	С	401	1PE	OH6-C15-C25-OH5



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Mol	Chain	Res	Type	Atoms
4	В	402	PG4	O1-C1-C2-O2
5	С	401	1PE	ОН7-С16-С26-ОН6
2	A	401	PEG	O1-C1-C2-O2
2	В	401	PEG	O1-C1-C2-O2
2	В	401	PEG	O2-C3-C4-O4
2	С	402	PEG	O1-C1-C2-O2
3	С	403	PGE	O3-C5-C6-O4
5	С	401	1PE	C12-C22-OH3-C23
4	В	402	PG4	O4-C7-C8-O5
5	С	401	1PE	C16-C26-OH6-C15
4	В	402	PG4	C3-C4-O3-C5
5	С	401	1PE	C23-C13-OH4-C24
2	С	402	PEG	C4-C3-O2-C2
2	С	402	PEG	C1-C2-O2-C3
2	A	401	PEG	C4-C3-O2-C2
4	В	402	PG4	C8-C7-O4-C6
3	A	402	PGE	C4-C3-O2-C2
3	A	402	PGE	C1-C2-O2-C3
4	В	402	PG4	O3-C5-C6-O4

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	PGE	2	0
2	В	401	PEG	1	0
2	С	402	PEG	1	0
5	С	401	1PE	1	0
3	С	403	PGE	1	0
4	В	402	PG4	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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9	
1	A	301/306 (98%)	0.08	3 (0%)	82	81	35, 49, 78, 93	0
1	В	304/306 (99%)	0.34	23 (7%)	13	11	36, 50, 86, 106	0
1	С	303/306 (99%)	-0.06	2 (0%)	87	86	35, 46, 71, 84	1 (0%)
All	All	908/918 (98%)	0.12	28 (3%)	49	45	35, 49, 79, 106	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	193	VAL	4.5
1	В	49	LEU	4.3
1	В	50	SER	3.7
1	В	25	MET	3.5
1	В	54	TYR	3.5
1	В	57	LEU	3.3
1	В	64	HIS	3.2
1	В	59	ILE	3.1
1	В	52	PRO	2.8
1	В	46	ALA	2.8
1	В	56	ALA	2.8
1	В	274	THR	2.6
1	В	45	PRO	2.6
1	В	51	ASP	2.6
1	В	77	ASN	2.6
1	С	303	VAL	2.5
1	В	61	MET	2.5
1	В	44	CYS	2.5
1	В	194	HIS	2.4
1	В	58	LEU	2.4
1	В	24	SER	2.4
1	В	192	GLN	2.4
1	A	57	LEU	2.3



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Mol	Chain	Res	Type	RSRZ
1	A	49	LEU	2.3
1	С	64	HIS	2.2
1	A	2	GLY	2.2
1	В	191	LYS	2.0
1	В	48	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	PGE	A	402	10/10	0.73	0.32	50,67,78,81	0
3	PGE	С	403	10/10	0.85	0.20	52,61,71,72	0
4	PG4	В	402	13/13	0.87	0.23	45,60,66,70	0
5	1PE	С	401	16/16	0.89	0.18	57,69,76,80	0
2	PEG	A	401	7/7	0.90	0.13	55,59,71,75	0
2	PEG	В	401	7/7	0.91	0.14	52,58,69,75	0
2	PEG	С	402	7/7	0.92	0.11	53,56,63,66	0

6.5 Other polymers (i)

There are no such residues in this entry.

