



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 02:23 PM GMT

PDB ID : 4IOX  
Title : The structure of the herpes simplex virus DNA-packaging motor pUL15 C-terminal nuclease domain provides insights into cleavage of concatemeric viral genome precursors  
Authors : Selvarajan Sigamani, S.; Zhao, H.; Kamau, Y.; Tang, L.  
Deposited on : 2013-01-08  
Resolution : 2.46 Å(reported)

This is a full wwPDB validation 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 <http://wwpdb.org/ValidationPDFNotes.html>

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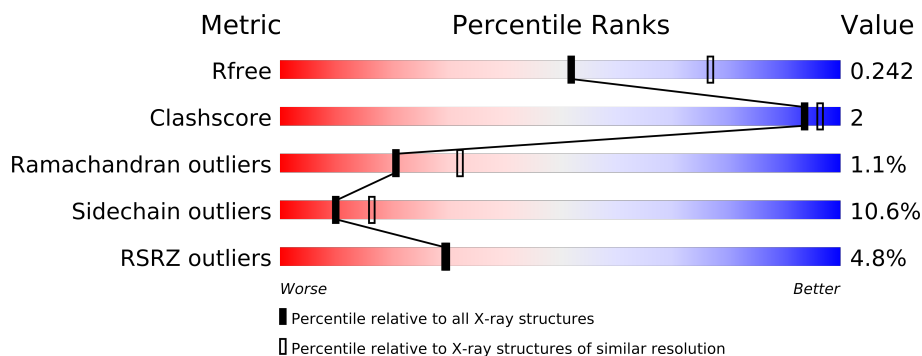
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.46 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))
$R_{free}$	66092	3566 (2.50-2.42)
Clashscore	79885	4471 (2.50-2.42)
Ramachandran outliers	78287	4383 (2.50-2.42)
Sidechain outliers	78261	4385 (2.50-2.42)
RSRZ outliers	66119	3568 (2.50-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	286	
1	B	286	
1	C	286	
2	D	6	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5172 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Tripartite terminase subunit UL15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1727	1109	295	316	7			
1	B	216	Total	C	N	O	S	0	0	0
			1653	1064	279	303	7			
1	C	220	Total	C	N	O	S	0	0	0
			1682	1085	283	307	7			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	MET	-	EXPRESSION TAG	UNP P04295
A	451	GLY	-	EXPRESSION TAG	UNP P04295
A	452	SER	-	EXPRESSION TAG	UNP P04295
A	453	SER	-	EXPRESSION TAG	UNP P04295
A	454	HIS	-	EXPRESSION TAG	UNP P04295
A	455	HIS	-	EXPRESSION TAG	UNP P04295
A	456	HIS	-	EXPRESSION TAG	UNP P04295
A	457	HIS	-	EXPRESSION TAG	UNP P04295
A	458	HIS	-	EXPRESSION TAG	UNP P04295
A	459	HIS	-	EXPRESSION TAG	UNP P04295
A	460	SER	-	EXPRESSION TAG	UNP P04295
A	461	SER	-	EXPRESSION TAG	UNP P04295
A	462	GLY	-	EXPRESSION TAG	UNP P04295
A	463	LEU	-	EXPRESSION TAG	UNP P04295
A	464	VAL	-	EXPRESSION TAG	UNP P04295
A	465	PRO	-	EXPRESSION TAG	UNP P04295
A	466	ARG	-	EXPRESSION TAG	UNP P04295
A	467	GLY	-	EXPRESSION TAG	UNP P04295
A	468	SER	-	EXPRESSION TAG	UNP P04295
A	469	HIS	-	EXPRESSION TAG	UNP P04295
A	470	MET	-	EXPRESSION TAG	UNP P04295
B	450	MET	-	EXPRESSION TAG	UNP P04295
B	451	GLY	-	EXPRESSION TAG	UNP P04295

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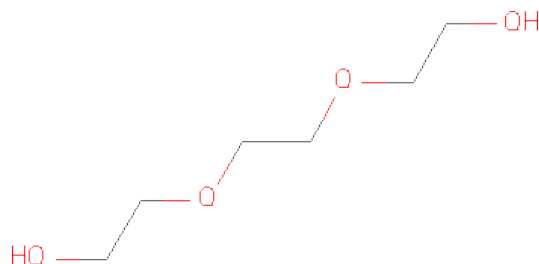
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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	SER	-	EXPRESSION TAG	UNP P04295
B	453	SER	-	EXPRESSION TAG	UNP P04295
B	454	HIS	-	EXPRESSION TAG	UNP P04295
B	455	HIS	-	EXPRESSION TAG	UNP P04295
B	456	HIS	-	EXPRESSION TAG	UNP P04295
B	457	HIS	-	EXPRESSION TAG	UNP P04295
B	458	HIS	-	EXPRESSION TAG	UNP P04295
B	459	HIS	-	EXPRESSION TAG	UNP P04295
B	460	SER	-	EXPRESSION TAG	UNP P04295
B	461	SER	-	EXPRESSION TAG	UNP P04295
B	462	GLY	-	EXPRESSION TAG	UNP P04295
B	463	LEU	-	EXPRESSION TAG	UNP P04295
B	464	VAL	-	EXPRESSION TAG	UNP P04295
B	465	PRO	-	EXPRESSION TAG	UNP P04295
B	466	ARG	-	EXPRESSION TAG	UNP P04295
B	467	GLY	-	EXPRESSION TAG	UNP P04295
B	468	SER	-	EXPRESSION TAG	UNP P04295
B	469	HIS	-	EXPRESSION TAG	UNP P04295
B	470	MET	-	EXPRESSION TAG	UNP P04295
C	450	MET	-	EXPRESSION TAG	UNP P04295
C	451	GLY	-	EXPRESSION TAG	UNP P04295
C	452	SER	-	EXPRESSION TAG	UNP P04295
C	453	SER	-	EXPRESSION TAG	UNP P04295
C	454	HIS	-	EXPRESSION TAG	UNP P04295
C	455	HIS	-	EXPRESSION TAG	UNP P04295
C	456	HIS	-	EXPRESSION TAG	UNP P04295
C	457	HIS	-	EXPRESSION TAG	UNP P04295
C	458	HIS	-	EXPRESSION TAG	UNP P04295
C	459	HIS	-	EXPRESSION TAG	UNP P04295
C	460	SER	-	EXPRESSION TAG	UNP P04295
C	461	SER	-	EXPRESSION TAG	UNP P04295
C	462	GLY	-	EXPRESSION TAG	UNP P04295
C	463	LEU	-	EXPRESSION TAG	UNP P04295
C	464	VAL	-	EXPRESSION TAG	UNP P04295
C	465	PRO	-	EXPRESSION TAG	UNP P04295
C	466	ARG	-	EXPRESSION TAG	UNP P04295
C	467	GLY	-	EXPRESSION TAG	UNP P04295
C	468	SER	-	EXPRESSION TAG	UNP P04295
C	469	HIS	-	EXPRESSION TAG	UNP P04295
C	470	MET	-	EXPRESSION TAG	UNP P04295

- Molecule 2 is a protein called peptide.

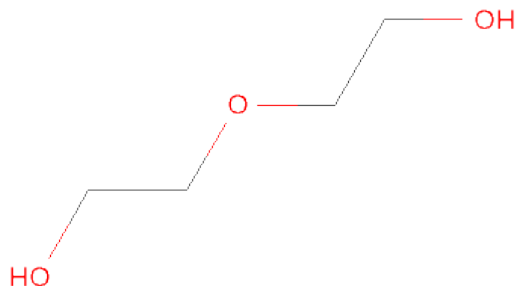
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	6	Total	C	N	O	0	0	0
			30	18	6	6			

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



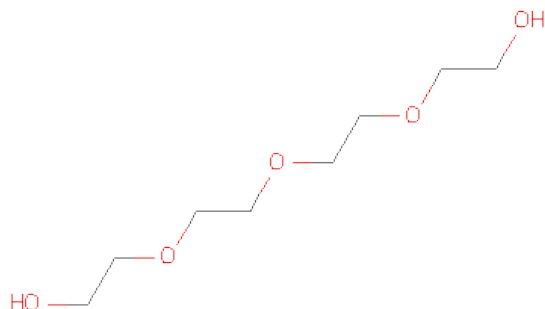
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

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



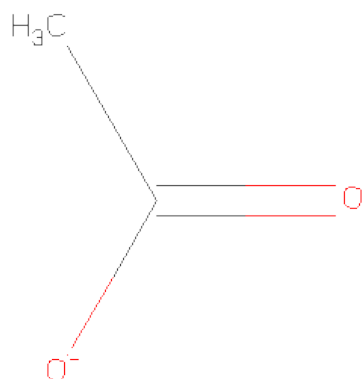
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	16	Total	O	0	0
			16	16		
7	B	21	Total	O	0	0
			21	21		
7	C	9	Total	O	0	0
			9	9		



- Molecule 2: peptide

Chain D:



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.94Å 96.94Å 194.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.46 33.75 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.80-2.46) 95.7 (33.75-2.46)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.01 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.203 , 0.247 0.204 , 0.242	Depositor DCC
$R_{free}$ test set	1654 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34365 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, PEG, PGE, ACT

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	0.48	0/1770	0.61	0/2412
1	B	0.49	0/1692	0.67	1/2303 (0.0%)
1	C	0.45	0/1722	0.61	0/2345
All	All	0.47	0/5184	0.63	1/7060 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	723	GLY	N-CA-C	9.96	138.00	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	721	GLN	Peptide
1	B	721	GLN	Peptide
1	B	723	GLY	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1727	0	0	5	0
1	B	1653	0	0	2	0
1	C	1682	0	0	1	0
2	D	30	0	0	0	0
3	A	10	0	0	0	0
4	A	7	0	0	0	0
5	A	13	0	0	0	0
6	A	4	0	0	0	0
7	A	16	0	0	2	0
7	B	21	0	0	0	0
7	C	9	0	0	0	0
All	All	5172	0	0	8	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (8) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:503:ASP:OD1	1:B:577:ARG:NH2	2.30	0.64
1:A:528:ARG:NH2	7:A:915:HOH:O	2.35	0.59
1:A:543:LEU:N	7:A:907:HOH:O	2.43	0.51
1:A:637:ASN:N	1:A:639:GLN:OE1	2.48	0.47
1:A:500:MET:O	1:A:727:THR:N	2.53	0.42
1:C:487:LEU:O	1:C:490:ARG:NE	2.53	0.40
1:B:487:LEU:O	1:B:490:ARG:NE	2.54	0.40
1:A:572:ALA:O	1:A:727:THR:OG1	2.40	0.40

There are no symmetry-related clashes.

## 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	219/286 (77%)	210 (96%)	8 (4%)	1 (0%)	38	57
1	B	206/286 (72%)	195 (95%)	8 (4%)	3 (2%)	15	23
1	C	210/286 (73%)	197 (94%)	10 (5%)	3 (1%)	16	25
All	All	635/858 (74%)	602 (95%)	26 (4%)	7 (1%)	21	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	730	PRO
1	C	730	PRO
1	B	724	PRO
1	B	725	PRO
1	C	724	PRO
1	A	724	PRO
1	C	725	PRO

### 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	184/233 (79%)	165 (90%)	19 (10%)	10	17
1	B	176/233 (76%)	155 (88%)	21 (12%)	8	12
1	C	179/233 (77%)	162 (90%)	17 (10%)	12	21
All	All	539/699 (77%)	482 (89%)	57 (11%)	10	16

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	480	LYS
1	A	488	LEU
1	A	504	LEU
1	A	506	VAL
1	A	508	VAL
1	A	517	ARG
1	A	525	VAL
1	A	561	SER
1	A	587	ASP
1	A	616	GLU
1	A	618	LEU
1	A	636	LEU
1	A	638	LYS
1	A	656	VAL
1	A	657	MET
1	A	661	GLU
1	A	708	LEU
1	A	721	GLN
1	A	727	THR
1	B	488	LEU
1	B	504	LEU
1	B	506	VAL
1	B	508	VAL
1	B	528	ARG
1	B	561	SER
1	B	562	LEU
1	B	576	VAL
1	B	602	ARG
1	B	618	LEU
1	B	623	GLU
1	B	629	VAL
1	B	636	LEU
1	B	639	GLN
1	B	650	LYS
1	B	656	VAL
1	B	657	MET
1	B	668	ARG
1	B	708	LEU
1	B	718	LEU
1	B	721	GLN
1	C	488	LEU
1	C	504	LEU
1	C	506	VAL

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Mol	Chain	Res	Type
1	C	508	VAL
1	C	564	GLN
1	C	576	VAL
1	C	577	ARG
1	C	585	SER
1	C	587	ASP
1	C	636	LEU
1	C	639	GLN
1	C	656	VAL
1	C	657	MET
1	C	661	GLU
1	C	708	LEU
1	C	718	LEU
1	C	721	GLN

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	PGE	A	801	-	9,9,9	0.61	0	8,8,8	1.38	0
4	PEG	A	802	-	6,6,6	0.57	0	5,5,5	1.33	0
5	PG4	A	803	-	12,12,12	0.69	0	11,11,11	1.36	0
6	ACT	A	804	-	1,3,3	1.24	0	0,3,3	0.00	-

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	801	-	-	0/7/7/7	0/0/0/0
4	PEG	A	802	-	-	0/4/4/4	0/0/0/0
5	PG4	A	803	-	-	0/10/10/10	0/0/0/0
6	ACT	A	804	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	225/286 (78%)	-0.12	6 (2%) 52 53	35, 49, 82, 114	0
1	B	216/286 (75%)	0.02	11 (5%) 27 27	35, 51, 87, 106	0
1	C	220/286 (76%)	0.26	15 (6%) 17 16	34, 54, 92, 121	0
2	D	0/6	-	-	-	-
All	All	661/864 (76%)	0.05	32 (4%) 29 30	34, 51, 87, 121	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	543	LEU	9.3
1	B	543	LEU	4.0
1	C	687	THR	3.9
1	B	548	GLY	3.9
1	B	542	PHE	3.6
1	C	728	PHE	3.5
1	B	728	PHE	3.3
1	A	517	ARG	3.2
1	C	723	GLY	3.1
1	B	613	SER	3.1
1	C	548	GLY	3.0
1	B	626	GLY	3.0
1	A	728	PHE	2.9
1	C	542	PHE	2.7
1	C	688	VAL	2.6
1	C	711	ALA	2.6
1	B	614	GLY	2.5
1	B	705	SER	2.3
1	B	616	GLU	2.3
1	C	626	GLY	2.3
1	A	620	TYR	2.3
1	C	477	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	629	VAL	2.2
1	A	722	ALA	2.2
1	C	541	PHE	2.1
1	C	712	VAL	2.1
1	C	638	LYS	2.1
1	B	731	ILE	2.1
1	C	549	SER	2.1
1	A	574	ARG	2.0
1	A	515	ASN	2.0
1	C	685	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PGE	A	801	10/10	0.20	1.74	50,61,69,73	0
6	ACT	A	804	4/4	0.18	1.19	78,85,87,90	0
5	PG4	A	803	13/13	0.22	0.83	66,80,86,88	0
4	PEG	A	802	7/7	0.13	-1.62	72,76,83,85	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.