



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:45 PM EDT

PDB ID : 5RD5  
Title : PanDDA analysis group deposition – Endothiapepsin ground state model 27  
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Deposited on : 2020-03-24  
Resolution : 1.15 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](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 : 2.10.1  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
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) : 2.10.1

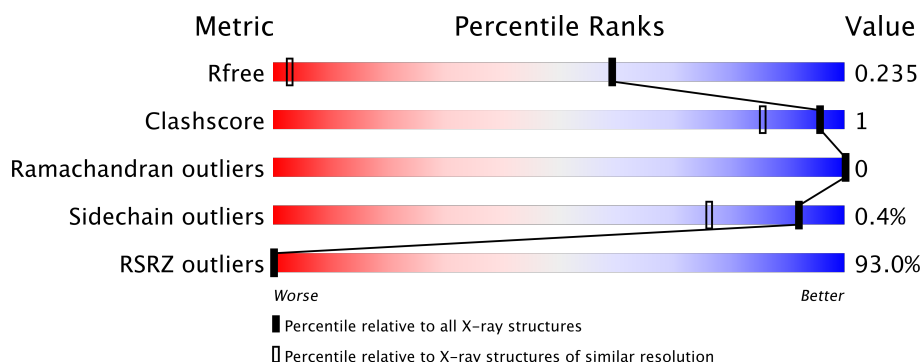
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.15 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))
$R_{free}$	111664	1223 (1.18-1.10)
Clashscore	122126	1264 (1.18-1.10)
Ramachandran outliers	120053	1215 (1.18-1.10)
Sidechain outliers	120020	1212 (1.18-1.10)
RSRZ outliers	108989	1199 (1.18-1.10)

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 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	419	<div> <div>73%</div> <div>78%</div> <div>21%</div> </div>

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
2	GOL	A	401	-	-	-	X
3	ACT	A	404[A]	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 2866 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 Endothiapepsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	19	0
			2462	1566	367	527	2			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



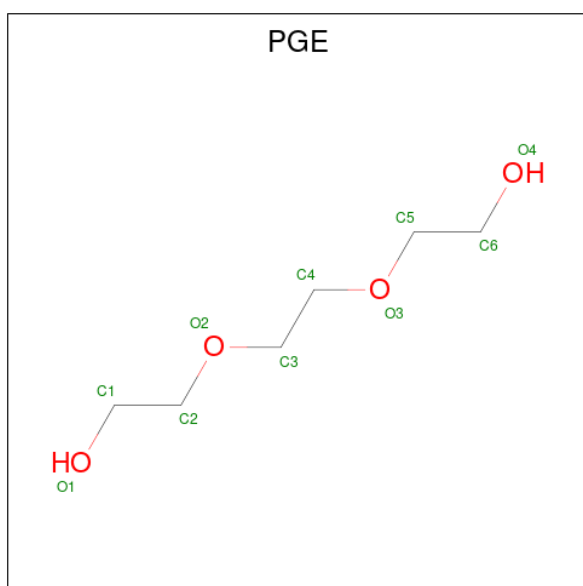
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	1
			12	6	6		
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

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



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

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

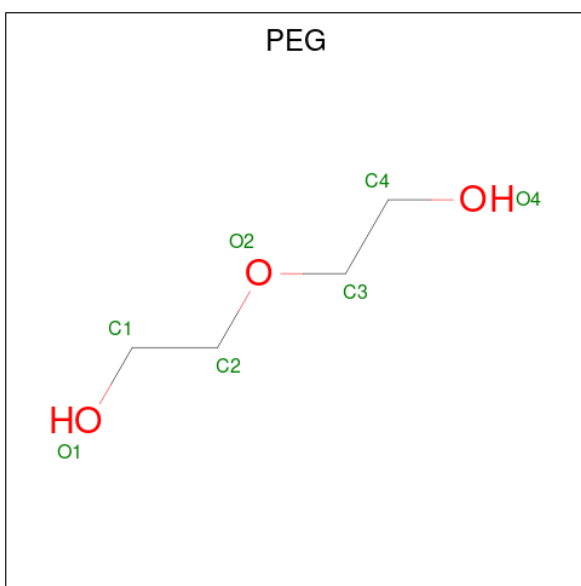


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 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
7	A	1	Total	C	O	0	0
			7	4	3		

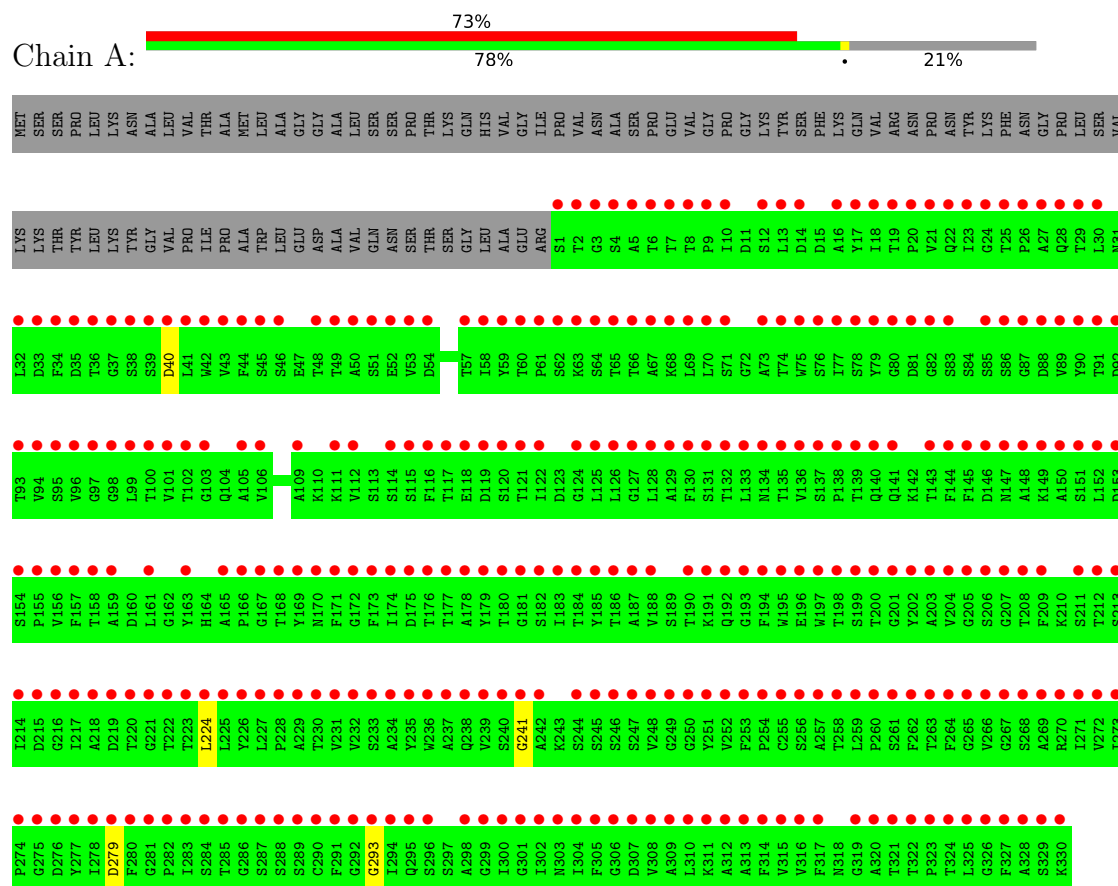
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	334	Total	O	0	9
			341	341		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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: Endothiapepsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.41 Å   72.86 Å   52.63 Å 90.00°   109.25°   90.00°	Depositor
Resolution (Å)	42.91 – 1.15 42.87 – 1.15	Depositor EDS
% Data completeness (in resolution range)	94.6 (42.91-1.15) 94.6 (42.87-1.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.95 (at 1.15 Å)	Xtriage
Refinement program	REFMAC 5.8.0238, PHENIX 1.16.3549	Depositor
R, $R_{free}$	0.238   ,   0.238 0.238   ,   0.235	Depositor DCC
$R_{free}$ test set	5281 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2866	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: GOL, PGE, NA, PG4, ACT, 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 angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.81	0/2552	0.94	0/3496

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2462	0	2329	5	0
2	A	24	0	32	4	0
3	A	8	0	6	1	0
4	A	10	0	14	0	0
5	A	13	0	18	0	0
6	A	1	0	0	0	0
7	A	7	0	10	0	0
8	A	341	0	0	1	1
All	All	2866	0	2409	6	1

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 (6) 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:A:241:GLY:H	2:A:403:GOL:H2	1.45	0.80
1:A:241:GLY:N	2:A:403:GOL:H2	2.11	0.64
1:A:279:ASP:OD1	3:A:405:ACT:H1	2.04	0.57
1:A:241:GLY:H	2:A:403:GOL:C2	2.21	0.47
2:A:402[B]:GOL:O3	8:A:501:HOH:O	2.21	0.44
1:A:224:LEU:HD22	1:A:293:GLY:HA2	2.01	0.42

All (1) 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)
8:A:512:HOH:O	8:A:781:HOH:O[1_556]	1.98	0.22

## 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	347/419 (83%)	344 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	270/336 (80%)	269 (100%)	1 (0%)	92 76

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP

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 molecules 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 ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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	$\# Z  > 2$
7	PEG	A	409	-	6,6,6	0.13	0	5,5,5	0.07	0
3	ACT	A	404[A]	-	1,3,3	3.53	1 (100%)	0,3,3	0.00	-
3	ACT	A	405	-	1,3,3	5.87	1 (100%)	0,3,3	0.00	-
2	GOL	A	402[B]	-	5,5,5	0.42	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	401	-	5,5,5	0.11	0	5,5,5	0.36	0
5	PG4	A	407	6	12,12,12	0.21	0	11,11,11	0.13	0
2	GOL	A	402[A]	-	5,5,5	0.09	0	5,5,5	0.28	0
4	PGE	A	406[A]	-	9,9,9	0.28	0	8,8,8	0.26	0
2	GOL	A	403	-	5,5,5	0.12	0	5,5,5	0.30	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
7	PEG	A	409	-	-	2/4/4/4	-
4	PGE	A	406[A]	-	-	1/7/7/7	-
2	GOL	A	402[B]	-	-	2/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
5	PG4	A	407	6	-	0/10/10/10	-
2	GOL	A	402[A]	-	-	1/4/4/4	-
2	GOL	A	403	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	ACT	CH3-C	5.87	1.56	1.48
3	A	404[A]	ACT	CH3-C	3.53	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402[B]	GOL	O1-C1-C2-C3
2	A	403	GOL	O1-C1-C2-C3
2	A	402[B]	GOL	O1-C1-C2-O2
2	A	403	GOL	O1-C1-C2-O2
2	A	402[A]	GOL	C1-C2-C3-O3
4	A	406[A]	PGE	O3-C5-C6-O4
2	A	403	GOL	O2-C2-C3-O3
7	A	409	PEG	C1-C2-O2-C3
7	A	409	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402[B]	GOL	1	0
2	A	403	GOL	3	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 ⓘ

### 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	330/419 (78%)	3.65	307 (93%) 0 0	10, 14, 22, 32	0

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	ALA	11.1
1	A	299[A]	GLY	8.4
1	A	300[A]	ILE	8.4
1	A	190	THR	7.6
1	A	94	VAL	7.2
1	A	80	GLY	7.0
1	A	23	ILE	6.7
1	A	325[A]	LEU	6.4
1	A	17	TYR	6.2
1	A	217	ILE	6.2
1	A	197	TRP	6.1
1	A	10	ILE	6.1
1	A	136	VAL	6.0
1	A	82	GLY	6.0
1	A	272	VAL	6.0
1	A	126	LEU	5.9
1	A	145	PHE	5.9
1	A	305	PHE	5.8
1	A	99	LEU	5.8
1	A	204	VAL	5.8
1	A	214	ILE	5.8
1	A	298[A]	ALA	5.8
1	A	74	THR	5.8
1	A	321	THR	5.8
1	A	236	TRP	5.7
1	A	37	GLY	5.7
1	A	138	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	294	ILE	5.6
1	A	109	ALA	5.4
1	A	76	SER	5.4
1	A	90	TYR	5.4
1	A	174[A]	ILE	5.3
1	A	193	GLY	5.3
1	A	30	LEU	5.3
1	A	310	LEU	5.3
1	A	139	THR	5.3
1	A	255	CYS	5.2
1	A	122	ILE	5.2
1	A	304	ILE	5.2
1	A	251	TYR	5.1
1	A	51	SER	5.1
1	A	78	SER	5.1
1	A	44	PHE	5.1
1	A	264	PHE	5.1
1	A	316	VAL	5.1
1	A	239	VAL	5.0
1	A	283	ILE	5.0
1	A	280	PHE	5.0
1	A	227	LEU	5.0
1	A	101	VAL	5.0
1	A	226	TYR	5.0
1	A	245	SER	4.9
1	A	42	TRP	4.9
1	A	224	LEU	4.9
1	A	195	TRP	4.9
1	A	267	GLY	4.9
1	A	234	ALA	4.9
1	A	102	THR	4.9
1	A	276[A]	ASP	4.9
1	A	246[A]	SER	4.9
1	A	50	ALA	4.8
1	A	225	LEU	4.8
1	A	188	VAL	4.8
1	A	6	THR	4.8
1	A	285	THR	4.8
1	A	163	TYR	4.8
1	A	185	TYR	4.8
1	A	209	PHE	4.7
1	A	133	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	183	ILE	4.7
1	A	91	THR	4.7
1	A	259	LEU	4.7
1	A	208	THR	4.7
1	A	9[A]	PRO	4.6
1	A	77	ILE	4.6
1	A	302	ILE	4.6
1	A	130	PHE	4.6
1	A	18	ILE	4.6
1	A	323	PRO	4.6
1	A	151	SER	4.6
1	A	194	PHE	4.5
1	A	128	LEU	4.5
1	A	143	THR	4.5
1	A	73	ALA	4.5
1	A	69	LEU	4.5
1	A	135	THR	4.5
1	A	248	VAL	4.4
1	A	114	SER	4.4
1	A	253	PHE	4.4
1	A	115	SER	4.4
1	A	263	THR	4.3
1	A	178	ALA	4.3
1	A	79	TYR	4.3
1	A	144	PHE	4.3
1	A	315	VAL	4.3
1	A	93	THR	4.3
1	A	278	ILE	4.3
1	A	134	ASN	4.2
1	A	173	PHE	4.2
1	A	41	LEU	4.2
1	A	129	ALA	4.2
1	A	244	SER	4.1
1	A	161	LEU	4.1
1	A	231	VAL	4.1
1	A	116	PHE	4.1
1	A	235	TYR	4.1
1	A	53	VAL	4.1
1	A	271	ILE	4.1
1	A	322	THR	4.0
1	A	237	ALA	4.0
1	A	100	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	159	ALA	4.0
1	A	200	THR	4.0
1	A	43	VAL	4.0
1	A	273	ILE	3.9
1	A	206[A]	SER	3.9
1	A	291	PHE	3.9
1	A	154[A]	SER	3.9
1	A	198	THR	3.9
1	A	327	PHE	3.9
1	A	98	GLY	3.9
1	A	16	ALA	3.8
1	A	232	VAL	3.8
1	A	158	THR	3.8
1	A	152	LEU	3.8
1	A	186	THR	3.8
1	A	290	CYS	3.8
1	A	105	ALA	3.8
1	A	328	ALA	3.8
1	A	75	TRP	3.8
1	A	96	VAL	3.8
1	A	7	THR	3.8
1	A	177	THR	3.8
1	A	34	PHE	3.8
1	A	215[A]	ASP	3.8
1	A	308	VAL	3.7
1	A	205	GLY	3.7
1	A	309	ALA	3.7
1	A	149[A]	LYS	3.7
1	A	89	VAL	3.7
1	A	125	LEU	3.7
1	A	58	ILE	3.7
1	A	49	THR	3.7
1	A	5	ALA	3.7
1	A	146	ASP	3.7
1	A	156	VAL	3.7
1	A	32	LEU	3.6
1	A	180	THR	3.6
1	A	62	SER	3.6
1	A	312	ALA	3.6
1	A	87	GLY	3.6
1	A	282	PRO	3.5
1	A	168	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	258	THR	3.5
1	A	70	LEU	3.5
1	A	262	PHE	3.5
1	A	182[A]	SER	3.5
1	A	132	THR	3.5
1	A	221	GLY	3.5
1	A	71[A]	SER	3.5
1	A	317	PHE	3.5
1	A	27	ALA	3.5
1	A	242	ALA	3.5
1	A	306	GLY	3.5
1	A	21	VAL	3.4
1	A	266	VAL	3.4
1	A	314	PHE	3.4
1	A	59	TYR	3.4
1	A	169	TYR	3.4
1	A	179	TYR	3.4
1	A	121	THR	3.4
1	A	229	ALA	3.4
1	A	257	ALA	3.3
1	A	60	THR	3.3
1	A	184	THR	3.3
1	A	127	GLY	3.3
1	A	252	VAL	3.3
1	A	260	PRO	3.3
1	A	36	THR	3.3
1	A	220	THR	3.3
1	A	148	ALA	3.3
1	A	165	ALA	3.3
1	A	35	ASP	3.3
1	A	65	THR	3.3
1	A	277	TYR	3.3
1	A	320	ALA	3.3
1	A	24	GLY	3.3
1	A	281	GLY	3.3
1	A	324	THR	3.3
1	A	171	PHE	3.2
1	A	25	THR	3.2
1	A	26	PRO	3.2
1	A	254	PRO	3.2
1	A	119	ASP	3.2
1	A	207	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	301	GLY	3.2
1	A	83	SER	3.2
1	A	187	ALA	3.1
1	A	203	ALA	3.1
1	A	274	PRO	3.1
1	A	175	ASP	3.1
1	A	106	VAL	3.1
1	A	238	GLN	3.1
1	A	230	THR	3.1
1	A	247	SER	3.1
1	A	45	SER	3.1
1	A	66	THR	3.1
1	A	176	THR	3.1
1	A	166	PRO	3.1
1	A	111	LYS	3.1
1	A	269	ALA	3.1
1	A	313	ALA	3.1
1	A	167	GLY	3.1
1	A	40	ASP	3.1
1	A	81	ASP	3.1
1	A	67	ALA	3.0
1	A	57	THR	3.0
1	A	20	PRO	3.0
1	A	13	LEU	3.0
1	A	14	ASP	3.0
1	A	172	GLY	3.0
1	A	286	GLY	3.0
1	A	287	SER	3.0
1	A	250	GLY	3.0
1	A	118	GLU	2.9
1	A	202	TYR	2.9
1	A	222	THR	2.9
1	A	86	SER	2.9
1	A	256	SER	2.9
1	A	288	SER	2.9
1	A	201	GLY	2.9
1	A	241	GLY	2.9
1	A	289[A]	SER	2.9
1	A	137	SER	2.9
1	A	218	ALA	2.9
1	A	33	ASP	2.8
1	A	141	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	29	THR	2.8
1	A	140	GLN	2.8
1	A	213	SER	2.8
1	A	228	PRO	2.8
1	A	157	PHE	2.8
1	A	2	THR	2.8
1	A	63	LYS	2.8
1	A	240[A]	SER	2.7
1	A	117	THR	2.7
1	A	223	THR	2.7
1	A	319	GLY	2.7
1	A	46	SER	2.7
1	A	284	SER	2.7
1	A	191	LYS	2.7
1	A	311[A]	LYS	2.7
1	A	95	SER	2.7
1	A	211	SER	2.7
1	A	296	SER	2.7
1	A	61	PRO	2.7
1	A	212	THR	2.7
1	A	216	GLY	2.7
1	A	293	GLY	2.7
1	A	19	THR	2.6
1	A	270	ARG	2.6
1	A	307	ASP	2.6
1	A	112	VAL	2.6
1	A	8	THR	2.6
1	A	155	PRO	2.5
1	A	326	GLY	2.5
1	A	22	GLN	2.5
1	A	292	GLY	2.5
1	A	170	ASN	2.5
1	A	1	SER	2.5
1	A	85	SER	2.5
1	A	261	SER	2.5
1	A	268[A]	SER	2.5
1	A	52	GLU	2.5
1	A	97	GLY	2.5
1	A	249	GLY	2.5
1	A	48	THR	2.5
1	A	275	GLY	2.5
1	A	88	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	120	SER	2.5
1	A	219	ASP	2.4
1	A	28	GLN	2.4
1	A	38	SER	2.4
1	A	68[A]	LYS	2.4
1	A	124	GLY	2.3
1	A	295	GLN	2.3
1	A	330	LYS	2.3
1	A	199	SER	2.3
1	A	4	SER	2.3
1	A	39	SER	2.3
1	A	92	ASP	2.3
1	A	181	GLY	2.3
1	A	303	ASN	2.2
1	A	3	GLY	2.2
1	A	103	GLY	2.2
1	A	147	ASN	2.2
1	A	131	SER	2.2
1	A	192	GLN	2.2
1	A	329	SER	2.1
1	A	153	ASP	2.1
1	A	265	GLY	2.1
1	A	12	SER	2.1
1	A	233	SER	2.1
1	A	54	ASP	2.1
1	A	279	ASP	2.1
1	A	64	SER	2.0
1	A	196	GLU	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 carbohydrates 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<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
5	PG4	A	407	13/13	0.39	0.28	36,41,51,52	0
2	GOL	A	402[B]	6/6	0.40	0.38	21,30,31,31	6
2	GOL	A	402[A]	6/6	0.40	0.38	20,22,23,25	6
3	ACT	A	405	4/4	0.53	0.21	25,26,29,31	0
7	PEG	A	409	7/7	0.54	0.38	47,47,50,55	0
3	ACT	A	404[A]	4/4	0.57	0.41	21,22,23,26	4
4	PGE	A	406[A]	10/10	0.61	0.29	26,30,37,40	10
6	NA	A	408	1/1	0.70	0.18	61,61,61,61	0
2	GOL	A	403	6/6	0.74	0.30	25,29,33,34	6
2	GOL	A	401	6/6	0.75	0.42	14,19,24,29	6

## 6.5 Other polymers [i](#)

There are no such residues in this entry.