



# Full wwPDB X-ray Structure Validation Report i

Aug 7, 2020 – 04:40 PM BST

PDB ID : 5RE3  
Title : PanDDA analysis group deposition – Endothiapepsin ground state model 12  
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Deposited on : 2020-03-24  
Resolution : 1.09 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 i symbol.

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The following versions of software and data (see [references](#) ①) 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 : 2.13.1  
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) : 2.13.1

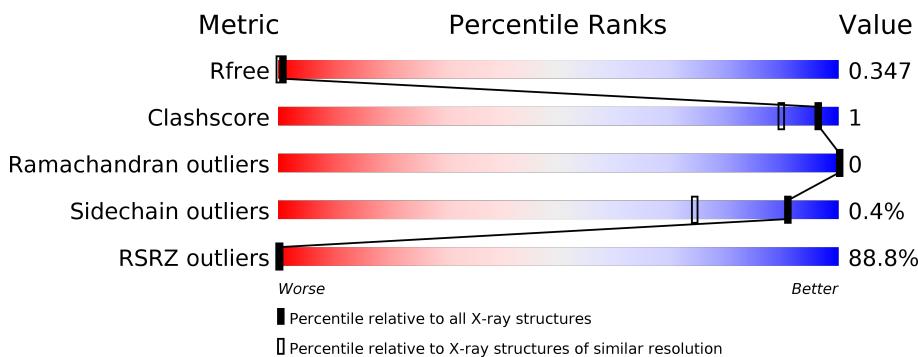
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

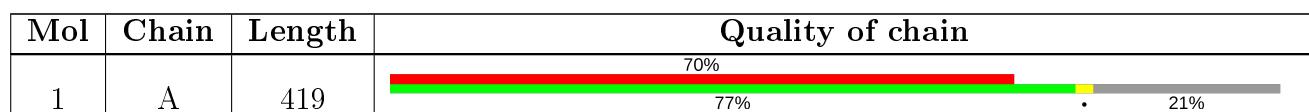
The reported resolution of this entry is 1.09 Å.

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	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

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 >=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.



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
3	ACT	A	404[A]	-	-	-	X

## 2 Entry composition (i)

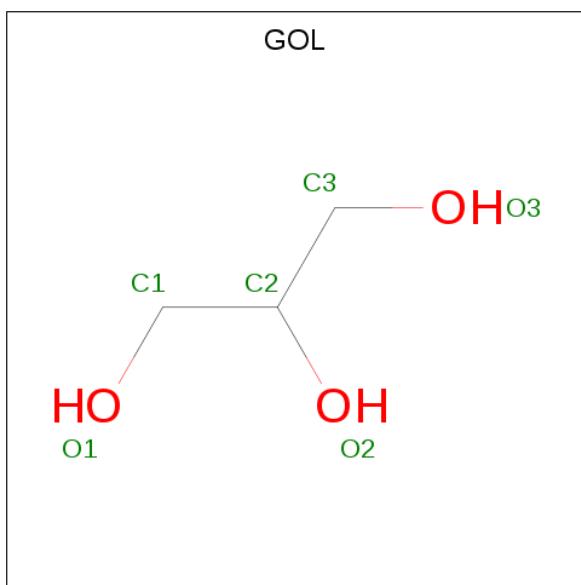
There are 7 unique types of molecules in this entry. The entry contains 2525 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

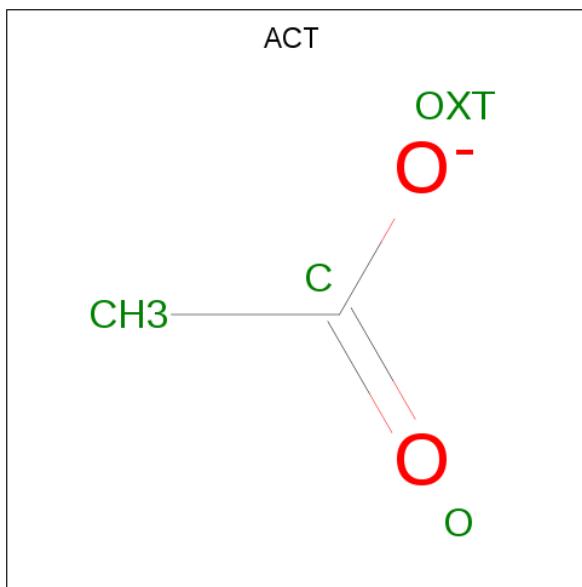
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2462	1566	367	527	2	0	19	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



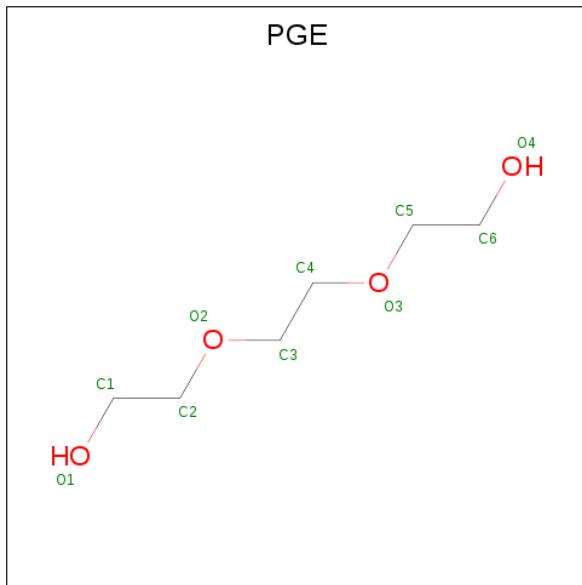
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	A	1	12	6	6	0	1
2	A	1	6	3	3	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



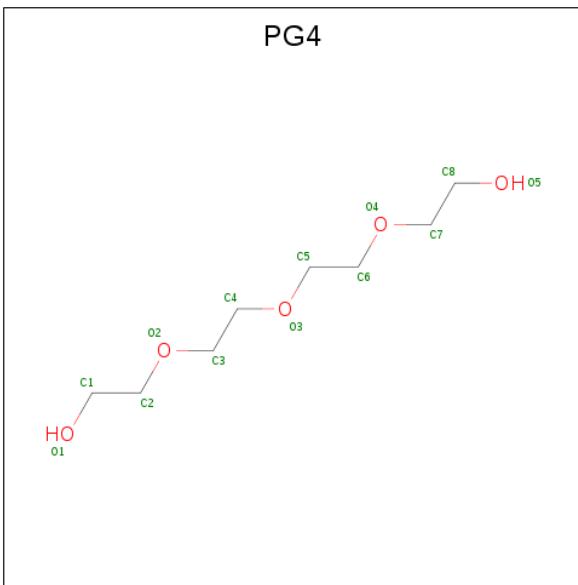
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	1
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).

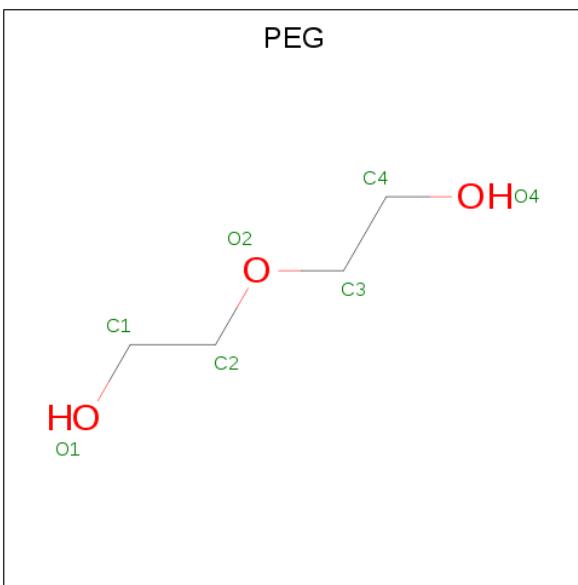


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	13	8	5	0	0

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

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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).

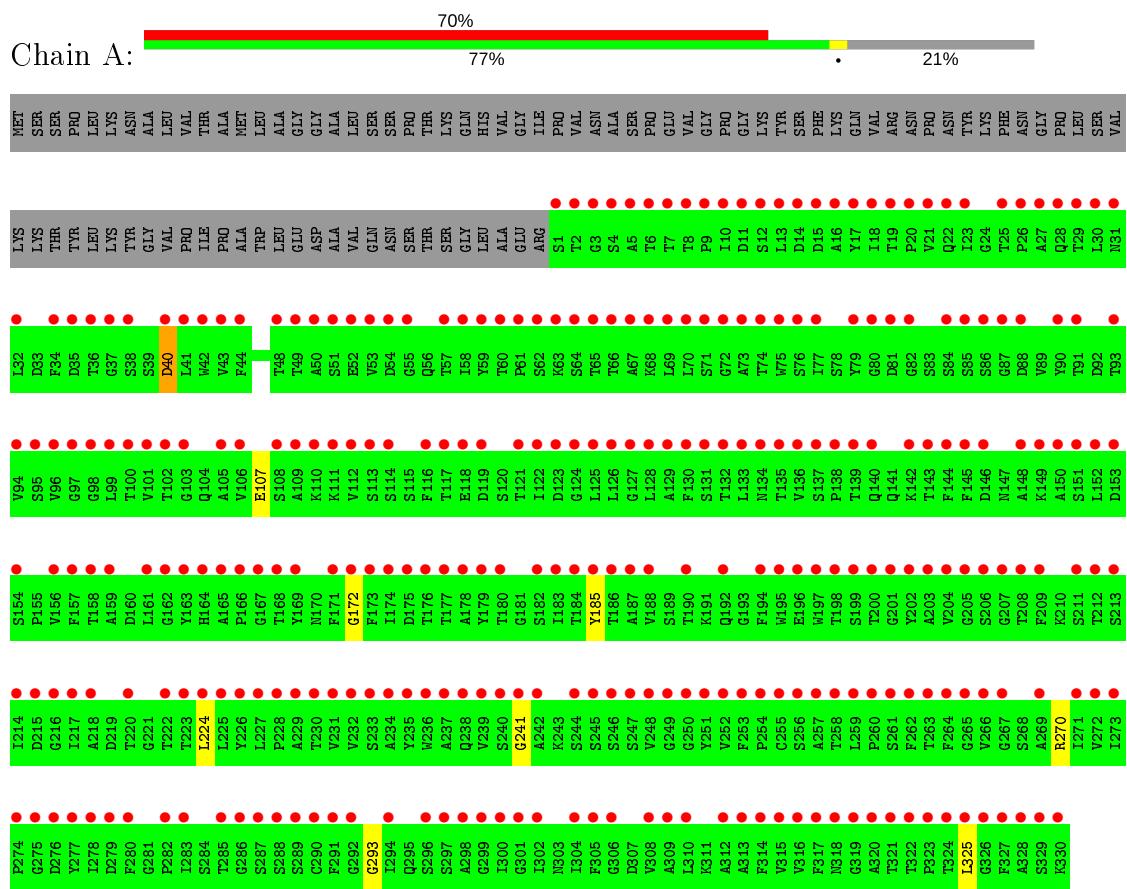


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		

### 3 Residue-property plots

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: Endothiapepsin



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.30 Å    72.87 Å    52.69 Å 90.00°    109.36°    90.00°	Depositor
Resolution (Å)	49.76 – 1.09 49.71 – 1.09	Depositor EDS
% Data completeness (in resolution range)	89.4 (49.76-1.09) 89.5 (49.71-1.09)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	0.98 (at 1.09 Å)	Xtriage
Refinement program	REFMAC 5.8.0238, PHENIX 1.16.3549	Depositor
$R$ , $R_{free}$	0.339 , 0.339 0.342 , 0.347	Depositor DCC
$R_{free}$ test set	5792 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.76 , 67.0	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.55$ , $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	2525	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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  $< |L| >$ ,  $< L^2 >$  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: 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	0.77	0/2552	0.92	1/3496 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	270	ARG	NE-CZ-NH1	5.55	123.08	120.30

There are no chirality outliers.

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	2462	0	2329	5	0
2	A	24	0	32	1	0
3	A	8	0	6	0	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
All	All	2525	0	2409	5	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 (5) 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:185:TYR:HA	1:A:325[A]:LEU:O	2.16	0.46
1:A:241:GLY:H	2:A:403:GOL:H2	1.81	0.46
1:A:224:LEU:HD22	1:A:293:GLY:HA2	1.97	0.46
1:A:40:ASP:OD2	1:A:107:GLU:OE2	2.38	0.42

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	347/419 (83%)	343 (99%)	4 (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%)	91 74

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 [\(i\)](#)

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 [\(i\)](#)

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$
2	GOL	A	401	-	5,5,5	0.12	0	5,5,5	0.43	0
2	GOL	A	402[B]	-	5,5,5	0.11	0	5,5,5	0.29	0
2	GOL	A	403	-	5,5,5	0.05	0	5,5,5	0.21	0
7	PEG	A	409	-	6,6,6	0.14	0	5,5,5	0.08	0
2	GOL	A	402[A]	-	5,5,5	0.08	0	5,5,5	0.21	0
3	ACT	A	404[A]	-	1,3,3	2.95	1 (100%)	0,3,3	0.00	-
4	PGE	A	406[A]	-	9,9,9	0.14	0	8,8,8	0.18	0
5	PG4	A	407	6	12,12,12	0.17	0	11,11,11	0.13	0
3	ACT	A	405	-	1,3,3	4.46	1 (100%)	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
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	A	402[B]	-	-	2/4/4/4	-
2	GOL	A	403	-	-	2/4/4/4	-
2	GOL	A	402[A]	-	-	0/4/4/4	-
7	PEG	A	409	-	-	1/4/4/4	-
5	PG4	A	407	6	-	1/10/10/10	-
4	PGE	A	406[A]	-	-	1/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	ACT	CH3-C	4.46	1.54	1.48
3	A	404[A]	ACT	CH3-C	2.95	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (7) 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	403	GOL	O1-C1-C2-O2
4	A	406[A]	PGE	O3-C5-C6-O4
2	A	402[B]	GOL	O1-C1-C2-O2
5	A	407	PG4	O4-C7-C8-O5
7	A	409	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	GOL	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<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%)	3.75	293 (88%) 0   0	9, 13, 20, 28	0

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	PRO	9.9
1	A	299[A]	GLY	9.5
1	A	80	GLY	9.5
1	A	197	TRP	9.1
1	A	176	THR	8.6
1	A	300[A]	ILE	8.5
1	A	130	PHE	8.4
1	A	58	ILE	8.2
1	A	174[A]	ILE	8.0
1	A	248	VAL	7.6
1	A	325[A]	LEU	7.0
1	A	285	THR	6.7
1	A	236	TRP	6.7
1	A	71[A]	SER	6.5
1	A	9[A]	PRO	6.4
1	A	48	THR	6.4
1	A	51	SER	6.4
1	A	319	GLY	6.4
1	A	184	THR	6.4
1	A	208	THR	6.4
1	A	173	PHE	6.3
1	A	198	THR	6.3
1	A	53	VAL	6.3
1	A	75	TRP	6.3
1	A	250	GLY	6.3
1	A	96	VAL	6.2
1	A	214	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	259	LEU	6.1
1	A	150	ALA	6.1
1	A	20	PRO	6.1
1	A	273	ILE	6.0
1	A	21	VAL	6.0
1	A	180	THR	6.0
1	A	290	CYS	5.9
1	A	4	SER	5.9
1	A	310	LEU	5.8
1	A	163	TYR	5.6
1	A	212	THR	5.6
1	A	249	GLY	5.6
1	A	30	LEU	5.5
1	A	253	PHE	5.5
1	A	283	ILE	5.5
1	A	133	LEU	5.5
1	A	171	PHE	5.4
1	A	166	PRO	5.4
1	A	316	VAL	5.4
1	A	280	PHE	5.4
1	A	73	ALA	5.4
1	A	54	ASP	5.3
1	A	23	ILE	5.3
1	A	16	ALA	5.3
1	A	241	GLY	5.3
1	A	94	VAL	5.3
1	A	136	VAL	5.3
1	A	93	THR	5.3
1	A	102	THR	5.3
1	A	139	THR	5.3
1	A	322	THR	5.3
1	A	77	ILE	5.2
1	A	195	TRP	5.2
1	A	41	LEU	5.1
1	A	143	THR	5.1
1	A	122	ILE	5.0
1	A	44	PHE	5.0
1	A	59	TYR	5.0
1	A	18	ILE	5.0
1	A	188	VAL	4.9
1	A	204	VAL	4.9
1	A	42	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	17	TYR	4.9
1	A	321	THR	4.9
1	A	70	LEU	4.9
1	A	161	LEU	4.9
1	A	320	ALA	4.8
1	A	232	VAL	4.8
1	A	111	LYS	4.8
1	A	101	VAL	4.8
1	A	112	VAL	4.8
1	A	272	VAL	4.8
1	A	329	SER	4.8
1	A	304	ILE	4.7
1	A	159	ALA	4.7
1	A	99	LEU	4.6
1	A	74	THR	4.6
1	A	291	PHE	4.6
1	A	69	LEU	4.6
1	A	183	ILE	4.6
1	A	294	ILE	4.6
1	A	2	THR	4.6
1	A	169	TYR	4.5
1	A	318	ASN	4.5
1	A	137	SER	4.5
1	A	324	THR	4.5
1	A	262	PHE	4.5
1	A	10	ILE	4.4
1	A	110	LYS	4.4
1	A	247	SER	4.4
1	A	302	ILE	4.4
1	A	308	VAL	4.4
1	A	121	THR	4.3
1	A	158	THR	4.3
1	A	215[A]	ASP	4.3
1	A	255	CYS	4.3
1	A	225	LEU	4.3
1	A	264	PHE	4.3
1	A	251	TYR	4.3
1	A	209	PHE	4.3
1	A	151	SER	4.2
1	A	79	TYR	4.2
1	A	26	PRO	4.2
1	A	146	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	222	THR	4.2
1	A	242	ALA	4.2
1	A	128	LEU	4.1
1	A	6	THR	4.1
1	A	34	PHE	4.1
1	A	186	THR	4.1
1	A	202	TYR	4.1
1	A	138	PRO	4.1
1	A	145	PHE	4.1
1	A	43	VAL	4.0
1	A	95	SER	4.0
1	A	76	SER	4.0
1	A	227	LEU	4.0
1	A	67	ALA	4.0
1	A	13	LEU	3.9
1	A	82	GLY	3.9
1	A	105	ALA	3.9
1	A	201	GLY	3.9
1	A	312	ALA	3.9
1	A	135	THR	3.9
1	A	327	PHE	3.9
1	A	315	VAL	3.9
1	A	144	PHE	3.9
1	A	275	GLY	3.8
1	A	5	ALA	3.8
1	A	98	GLY	3.8
1	A	199	SER	3.8
1	A	200	THR	3.7
1	A	206[A]	SER	3.7
1	A	90	TYR	3.7
1	A	109	ALA	3.7
1	A	246[A]	SER	3.7
1	A	172	GLY	3.7
1	A	81	ASP	3.7
1	A	157	PHE	3.7
1	A	38	SER	3.7
1	A	185	TYR	3.6
1	A	313	ALA	3.6
1	A	11	ASP	3.6
1	A	271	ILE	3.6
1	A	7	THR	3.6
1	A	194	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	177	THR	3.6
1	A	224	LEU	3.6
1	A	49	THR	3.5
1	A	106	VAL	3.5
1	A	244	SER	3.5
1	A	254	PRO	3.5
1	A	27	ALA	3.5
1	A	231	VAL	3.5
1	A	252	VAL	3.5
1	A	124	GLY	3.5
1	A	167	GLY	3.5
1	A	100	THR	3.5
1	A	190	THR	3.5
1	A	226	TYR	3.5
1	A	235	TYR	3.5
1	A	286	GLY	3.5
1	A	114	SER	3.4
1	A	258	THR	3.4
1	A	19	THR	3.4
1	A	277	TYR	3.4
1	A	228	PRO	3.4
1	A	168	THR	3.4
1	A	263	THR	3.4
1	A	305	PHE	3.4
1	A	297	SER	3.4
1	A	179	TYR	3.4
1	A	234	ALA	3.4
1	A	61	PRO	3.4
1	A	317	PHE	3.4
1	A	72	GLY	3.3
1	A	175	ASP	3.3
1	A	256	SER	3.3
1	A	29	THR	3.3
1	A	31	ASN	3.3
1	A	32	LEU	3.3
1	A	274	PRO	3.3
1	A	91	THR	3.3
1	A	240[A]	SER	3.2
1	A	152	LEU	3.2
1	A	149[A]	LYS	3.2
1	A	131	SER	3.2
1	A	117	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	64	SER	3.2
1	A	108	SER	3.2
1	A	182[A]	SER	3.2
1	A	237	ALA	3.1
1	A	314	PHE	3.1
1	A	217	ILE	3.1
1	A	8	THR	3.1
1	A	118	GLU	3.1
1	A	153	ASP	3.1
1	A	239	VAL	3.1
1	A	63	LYS	3.1
1	A	113	SER	3.0
1	A	116	PHE	3.0
1	A	164	HIS	3.0
1	A	238	GLN	3.0
1	A	129	ALA	3.0
1	A	289[A]	SER	3.0
1	A	156	VAL	3.0
1	A	326	GLY	3.0
1	A	296	SER	3.0
1	A	165	ALA	3.0
1	A	298[A]	ALA	3.0
1	A	288	SER	3.0
1	A	203	ALA	2.9
1	A	97	GLY	2.9
1	A	12	SER	2.9
1	A	220	THR	2.9
1	A	126	LEU	2.9
1	A	57	THR	2.9
1	A	62	SER	2.9
1	A	266	VAL	2.9
1	A	192	GLN	2.9
1	A	330	LYS	2.9
1	A	265	GLY	2.8
1	A	25	THR	2.8
1	A	50	ALA	2.8
1	A	86	SER	2.8
1	A	301	GLY	2.8
1	A	223	THR	2.8
1	A	230	THR	2.8
1	A	36	THR	2.7
1	A	125	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	278	ILE	2.7
1	A	119	ASP	2.7
1	A	213	SER	2.7
1	A	245	SER	2.7
1	A	282	PRO	2.7
1	A	267	GLY	2.7
1	A	205	GLY	2.6
1	A	207	GLY	2.6
1	A	328	ALA	2.6
1	A	55	GLY	2.6
1	A	162	GLY	2.6
1	A	60	THR	2.6
1	A	68[A]	LYS	2.6
1	A	37	GLY	2.5
1	A	276[A]	ASP	2.5
1	A	233	SER	2.5
1	A	134	ASN	2.5
1	A	1	SER	2.5
1	A	15	ASP	2.5
1	A	132	THR	2.5
1	A	187	ALA	2.4
1	A	309	ALA	2.4
1	A	260	PRO	2.4
1	A	88	ASP	2.4
1	A	269	ALA	2.4
1	A	154[A]	SER	2.4
1	A	65	THR	2.4
1	A	22	GLN	2.4
1	A	229	ALA	2.4
1	A	52	GLU	2.3
1	A	28	GLN	2.3
1	A	123	ASP	2.3
1	A	306	GLY	2.3
1	A	292	GLY	2.2
1	A	84	SER	2.2
1	A	66	THR	2.2
1	A	178	ALA	2.2
1	A	257	ALA	2.2
1	A	85	SER	2.2
1	A	127	GLY	2.2
1	A	148	ALA	2.2
1	A	218	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	142	LYS	2.1
1	A	87	GLY	2.1
1	A	196	GLU	2.1
1	A	14	ASP	2.1
1	A	216	GLY	2.1
1	A	287	SER	2.1
1	A	3	GLY	2.1
1	A	261	SER	2.0
1	A	103	GLY	2.0
1	A	35	ASP	2.0
1	A	279	ASP	2.0
1	A	211	SER	2.0
1	A	140	GLN	2.0
1	A	40	ASP	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<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
3	ACT	A	404[A]	4/4	0.11	0.57	21,22,23,23	4
7	PEG	A	409	7/7	0.14	0.38	53,55,56,56	0
6	NA	A	408	1/1	0.41	0.20	56,56,56,56	0
5	PG4	A	407	13/13	0.43	0.25	36,37,39,39	0
2	GOL	A	402[B]	6/6	0.48	0.38	18,23,23,25	6
2	GOL	A	402[A]	6/6	0.48	0.38	18,20,21,21	6
3	ACT	A	405	4/4	0.58	0.17	25,26,27,28	0
4	PGE	A	406[A]	10/10	0.62	0.28	32,33,35,35	10
2	GOL	A	403	6/6	0.63	0.33	25,30,31,31	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	A	401	6/6	0.81	0.21	14,17,19,22	6

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.