



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:07 AM UTC

PDB ID : 5RD5 / pdb_00005rd5
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

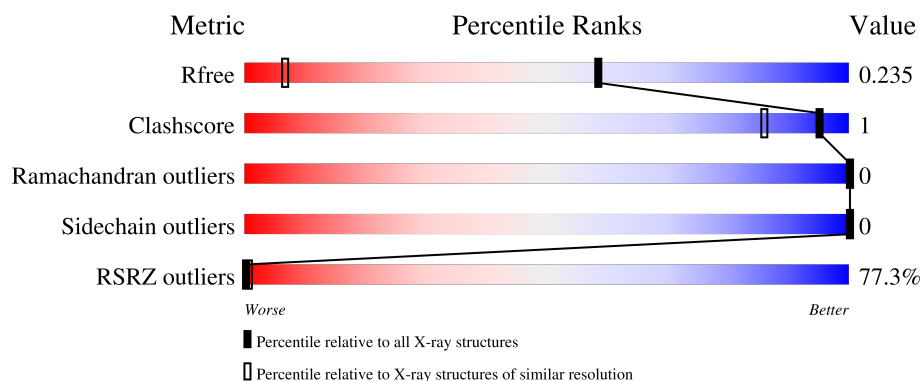
1 Overall quality at a glance

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}	180053	1380 (1.16-1.12)
Clashscore	190562	1393 (1.16-1.12)
Ramachandran outliers	187476	1369 (1.16-1.12)
Sidechain outliers	187428	1369 (1.16-1.12)
RSRZ outliers	180081	1379 (1.16-1.12)

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 $\leq 5\%$. 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	

2 Entry composition [i](#)

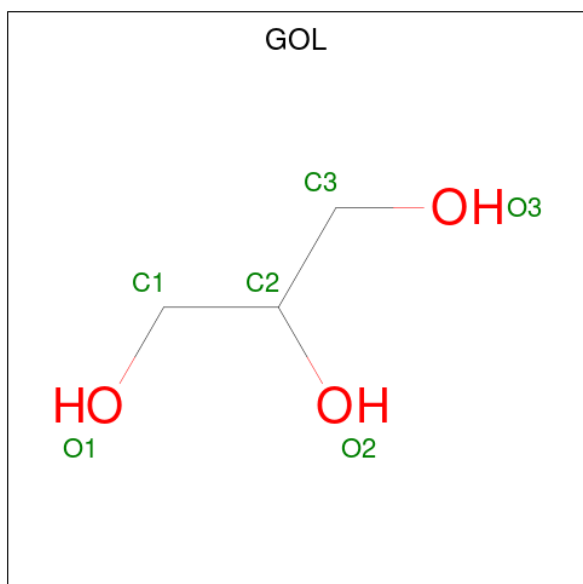
There are 8 unique types of molecules in this entry. The entry contains 2866 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

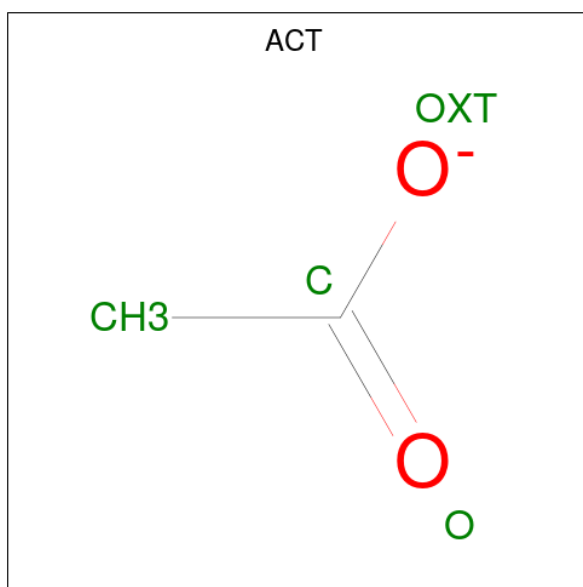
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	19	0
			2462	1566	367	527	2			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



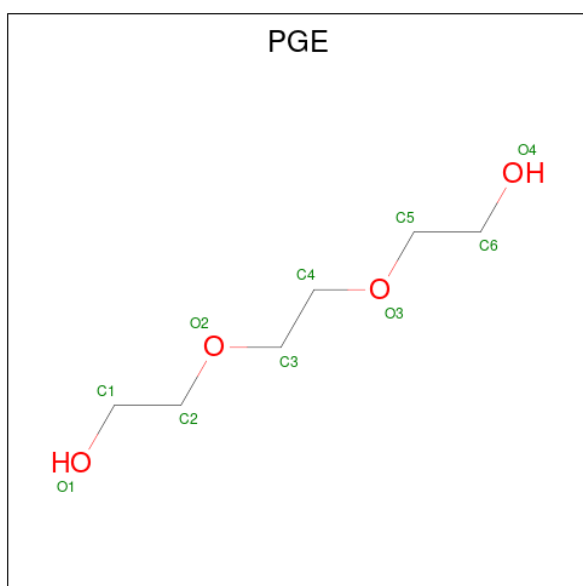
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	1
			12	6	6		
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



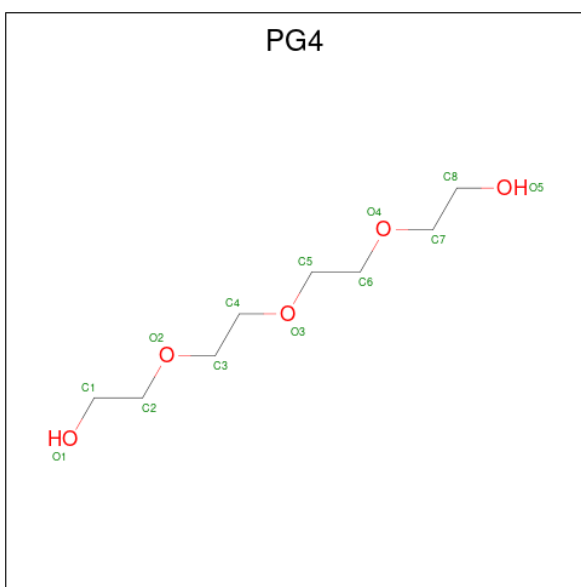
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: 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 (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

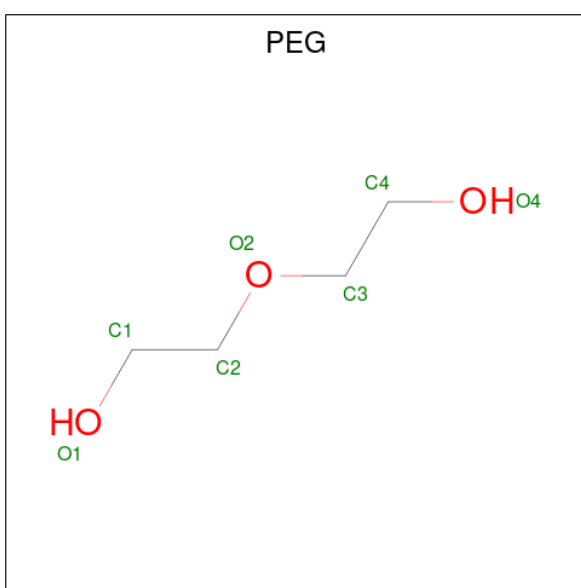


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.41 Å 72.86 Å 52.63 Å 90.00° 109.25° 90.00°	Depositor
Resolution (Å)	42.91 – 1.15 42.91 – 1.15	Depositor EDS
% Data completeness (in resolution range)	94.6 (42.91-1.15) 94.6 (42.91-1.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2866	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, GOL, PEG, PG4, NA, 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	1.13	3/2552 (0.1%)	1.17	2/3496 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	ILE	C-O	5.64	1.29	1.24
1	A	147	ASN	C-O	5.37	1.30	1.24
1	A	127	GLY	C-O	-5.16	1.18	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	PHE	CA-CB-CG	-6.18	107.62	113.80
1	A	322	THR	CB-CA-C	5.55	115.44	110.44

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	4	0
3	A	8	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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	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%)	270 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	31	ASN
1	A	164	HIS
1	A	303	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	402[A]	-	5,5,5	0.09	0	5,5,5	0.28	0
2	GOL	A	402[B]	-	5,5,5	0.44	0	5,5,5	0.36	0
5	PG4	A	407	6	12,12,12	0.20	0	11,11,11	0.12	0
7	PEG	A	409	-	6,6,6	0.13	0	5,5,5	0.07	0
2	GOL	A	401	-	5,5,5	0.11	0	5,5,5	0.37	0
2	GOL	A	403	-	5,5,5	0.13	0	5,5,5	0.30	0
3	ACT	A	404[A]	-	3,3,3	1.01	0	3,3,3	0.69	0
3	ACT	A	405	-	3,3,3	1.35	0	3,3,3	0.77	0
4	PGE	A	406[A]	-	9,9,9	0.29	0	8,8,8	0.26	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	GOL	A	402[A]	-	-	1/4/4/4	-
2	GOL	A	402[B]	-	-	2/4/4/4	-
5	PG4	A	407	6	-	0/10/10/10	-
7	PEG	A	409	-	-	2/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	A	403	-	-	3/4/4/4	-
4	PGE	A	406[A]	-	-	1/7/7/7	-

There are no bond length outliers.

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

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Mol	Chain	Res	Type	Atoms
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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402[B]	GOL	1	0
2	A	403	GOL	3	0
3	A	405	ACT	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

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, 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	330/419 (78%)	3.18	255 (77%) 0 1	6, 14, 22, 32	19 (5%)

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	ALA	9.5
1	A	300[A]	ILE	9.3
1	A	245	SER	8.1
1	A	321	THR	7.9
1	A	94	VAL	7.6
1	A	82	GLY	7.6
1	A	17	TYR	7.3
1	A	53	VAL	6.8
1	A	299[A]	GLY	6.6
1	A	10	ILE	6.5
1	A	214	ILE	6.5
1	A	248	VAL	6.4
1	A	258	THR	6.4
1	A	302	ILE	6.1
1	A	109	ALA	5.9
1	A	323	PRO	5.9
1	A	211	SER	5.8
1	A	325[A]	LEU	5.8
1	A	154[A]	SER	5.7
1	A	116	PHE	5.7
1	A	280	PHE	5.7
1	A	50	ALA	5.7
1	A	152	LEU	5.3
1	A	122	ILE	5.3
1	A	246[A]	SER	5.2
1	A	285	THR	5.2
1	A	132	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	212	THR	5.2
1	A	320	ALA	5.1
1	A	138	PRO	5.1
1	A	244	SER	4.9
1	A	190	THR	4.9
1	A	251	TYR	4.9
1	A	130	PHE	4.9
1	A	264	PHE	4.9
1	A	283	ILE	4.9
1	A	117	THR	4.8
1	A	90	TYR	4.8
1	A	217	ILE	4.8
1	A	193	GLY	4.8
1	A	151	SER	4.7
1	A	145	PHE	4.7
1	A	209	PHE	4.7
1	A	305	PHE	4.6
1	A	221	GLY	4.6
1	A	322	THR	4.6
1	A	13	LEU	4.6
1	A	200	THR	4.6
1	A	197	TRP	4.6
1	A	58	ILE	4.5
1	A	313	ALA	4.5
1	A	79	TYR	4.5
1	A	143	THR	4.5
1	A	178	ALA	4.5
1	A	46	SER	4.4
1	A	306	GLY	4.4
1	A	319	GLY	4.4
1	A	49	THR	4.4
1	A	119	ASP	4.4
1	A	242	ALA	4.4
1	A	236	TRP	4.3
1	A	99	LEU	4.3
1	A	176	THR	4.3
1	A	87	GLY	4.3
1	A	180	THR	4.2
1	A	121	THR	4.2
1	A	42	TRP	4.2
1	A	255	CYS	4.2
1	A	257	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	239	VAL	4.2
1	A	71[A]	SER	4.1
1	A	91	THR	4.1
1	A	52	GLU	4.1
1	A	66	THR	4.1
1	A	272	VAL	4.1
1	A	208	THR	4.0
1	A	179	TYR	4.0
1	A	308	VAL	4.0
1	A	177	THR	4.0
1	A	23	ILE	4.0
1	A	112	VAL	4.0
1	A	136	VAL	4.0
1	A	41	LEU	4.0
1	A	161	LEU	4.0
1	A	298[A]	ALA	4.0
1	A	44	PHE	3.9
1	A	327	PHE	3.9
1	A	16	ALA	3.9
1	A	65	THR	3.9
1	A	149[A]	LYS	3.9
1	A	75	TRP	3.9
1	A	301	GLY	3.9
1	A	30	LEU	3.9
1	A	155	PRO	3.8
1	A	135	THR	3.8
1	A	80	GLY	3.8
1	A	267	GLY	3.8
1	A	74	THR	3.8
1	A	162	GLY	3.8
1	A	48	THR	3.7
1	A	249	GLY	3.7
1	A	186	THR	3.7
1	A	250	GLY	3.7
1	A	67	ALA	3.7
1	A	163	TYR	3.7
1	A	9[A]	PRO	3.7
1	A	139	THR	3.7
1	A	201	GLY	3.7
1	A	114	SER	3.7
1	A	284	SER	3.7
1	A	171	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	77	ILE	3.6
1	A	156	VAL	3.6
1	A	133	LEU	3.6
1	A	45	SER	3.6
1	A	206[A]	SER	3.6
1	A	304	ILE	3.6
1	A	12	SER	3.5
1	A	61	PRO	3.5
1	A	115	SER	3.5
1	A	194	PHE	3.5
1	A	227	LEU	3.5
1	A	100	THR	3.5
1	A	102	THR	3.5
1	A	76	SER	3.4
1	A	72	GLY	3.4
1	A	106	VAL	3.4
1	A	62	SER	3.4
1	A	166	PRO	3.4
1	A	271	ILE	3.4
1	A	40	ASP	3.4
1	A	93	THR	3.4
1	A	101	VAL	3.4
1	A	126	LEU	3.4
1	A	266	VAL	3.4
1	A	253	PHE	3.3
1	A	195	TRP	3.3
1	A	309	ALA	3.3
1	A	81	ASP	3.3
1	A	204	VAL	3.3
1	A	281	GLY	3.3
1	A	134	ASN	3.3
1	A	26	PRO	3.3
1	A	63	LYS	3.3
1	A	83	SER	3.3
1	A	328	ALA	3.3
1	A	256	SER	3.2
1	A	247	SER	3.2
1	A	43	VAL	3.2
1	A	60	THR	3.2
1	A	185	TYR	3.2
1	A	146	ASP	3.1
1	A	105	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	129	ALA	3.1
1	A	269	ALA	3.1
1	A	329	SER	3.1
1	A	2	THR	3.1
1	A	238	GLN	3.1
1	A	207	GLY	3.1
1	A	54	ASP	3.1
1	A	263	THR	3.1
1	A	1	SER	3.1
1	A	78	SER	3.1
1	A	268[A]	SER	3.1
1	A	290	CYS	3.0
1	A	202	TYR	3.0
1	A	173	PHE	3.0
1	A	113	SER	3.0
1	A	86	SER	3.0
1	A	231	VAL	3.0
1	A	25	THR	3.0
1	A	218	ALA	3.0
1	A	234	ALA	3.0
1	A	224	LEU	3.0
1	A	164	HIS	2.9
1	A	59	TYR	2.9
1	A	158	THR	2.9
1	A	293	GLY	2.9
1	A	188	VAL	2.9
1	A	125	LEU	2.8
1	A	174[A]	ILE	2.8
1	A	291	PHE	2.8
1	A	314	PHE	2.8
1	A	169	TYR	2.8
1	A	69	LEU	2.8
1	A	183	ILE	2.8
1	A	240[A]	SER	2.7
1	A	37	GLY	2.7
1	A	157	PHE	2.7
1	A	51	SER	2.7
1	A	228	PRO	2.7
1	A	27	ALA	2.7
1	A	73	ALA	2.7
1	A	203	ALA	2.7
1	A	144	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	98	GLY	2.7
1	A	127	GLY	2.7
1	A	286	GLY	2.7
1	A	259	LEU	2.6
1	A	310	LEU	2.6
1	A	294	ILE	2.6
1	A	277	TYR	2.6
1	A	330	LYS	2.6
1	A	131	SER	2.6
1	A	88	ASP	2.6
1	A	31	ASN	2.6
1	A	128	LEU	2.5
1	A	241	GLY	2.5
1	A	254	PRO	2.5
1	A	318	ASN	2.5
1	A	6	THR	2.5
1	A	165	ALA	2.5
1	A	215[A]	ASP	2.5
1	A	167	GLY	2.5
1	A	175	ASP	2.5
1	A	182[A]	SER	2.4
1	A	118	GLU	2.4
1	A	39	SER	2.4
1	A	84	SER	2.4
1	A	192	GLN	2.4
1	A	34	PHE	2.4
1	A	168	THR	2.4
1	A	184	THR	2.4
1	A	15	ASP	2.4
1	A	226	TYR	2.4
1	A	5	ALA	2.4
1	A	237	ALA	2.4
1	A	8	THR	2.4
1	A	273	ILE	2.4
1	A	282	PRO	2.3
1	A	95	SER	2.3
1	A	153	ASP	2.3
1	A	159	ALA	2.3
1	A	85	SER	2.3
1	A	47	GLU	2.3
1	A	278	ILE	2.3
1	A	36	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	111	LYS	2.2
1	A	55	GLY	2.2
1	A	307	ASP	2.2
1	A	28	GLN	2.2
1	A	316	VAL	2.2
1	A	35	ASP	2.2
1	A	270	ARG	2.1
1	A	120	SER	2.1
1	A	198	THR	2.1
1	A	324	THR	2.1
1	A	92	ASP	2.1
1	A	89	VAL	2.1
1	A	170	ASN	2.1
1	A	276[A]	ASP	2.1
1	A	232	VAL	2.1
1	A	20	PRO	2.1
1	A	315	VAL	2.0
1	A	262	PHE	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 oligosaccharides 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
7	PEG	A	409	7/7	0.53	0.37	47,47,50,55	0
3	ACT	A	404[A]	4/4	0.56	0.30	21,22,23,26	4
5	PG4	A	407	13/13	0.59	0.33	36,41,51,52	0
3	ACT	A	405	4/4	0.61	0.23	25,26,29,31	0
4	PGE	A	406[A]	10/10	0.62	0.34	26,30,37,40	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	403	6/6	0.65	0.29	25,29,33,34	6
2	GOL	A	402[A]	6/6	0.71	0.27	20,22,23,25	6
2	GOL	A	402[B]	6/6	0.71	0.27	21,30,31,31	6
6	NA	A	408	1/1	0.76	0.26	61,61,61,61	0
2	GOL	A	401	6/6	0.81	0.27	14,19,24,29	6

6.5 Other polymers [i](#)

There are no such residues in this entry.