



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:30 AM UTC

PDB ID : 5RE3 / pdb_00005re3
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

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

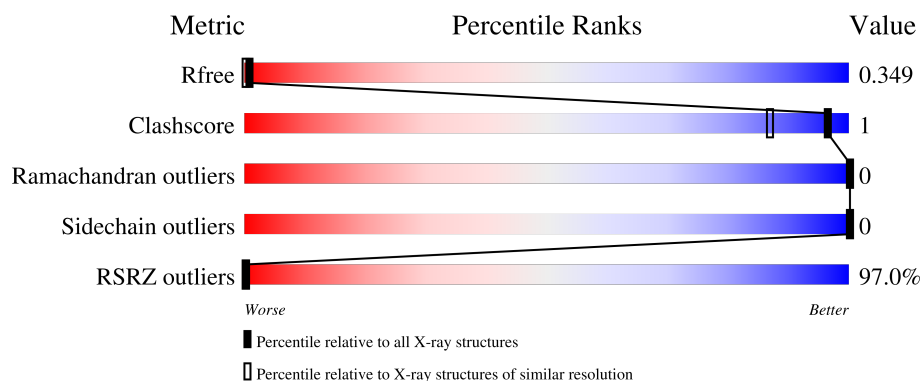
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.09 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}	180053	1625 (1.12-1.08)
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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	76% 76% 21%

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	403	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	404[A]	-	-	-	X
4	PGE	A	406[A]	-	-	-	X
6	NA	A	408	-	-	-	X
7	PEG	A	409	-	-	-	X

2 Entry composition [i](#)

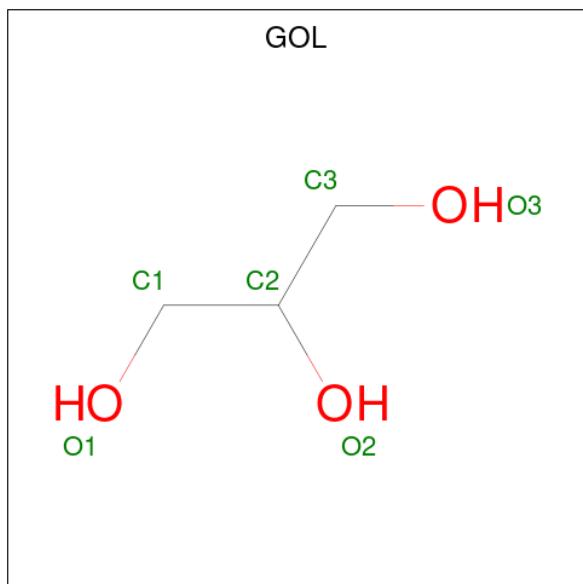
There are 7 unique types of molecules in this entry. The entry contains 2525 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	330	Total	C	N	O	S	0	19	0
			2462	1566	367	527	2			

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



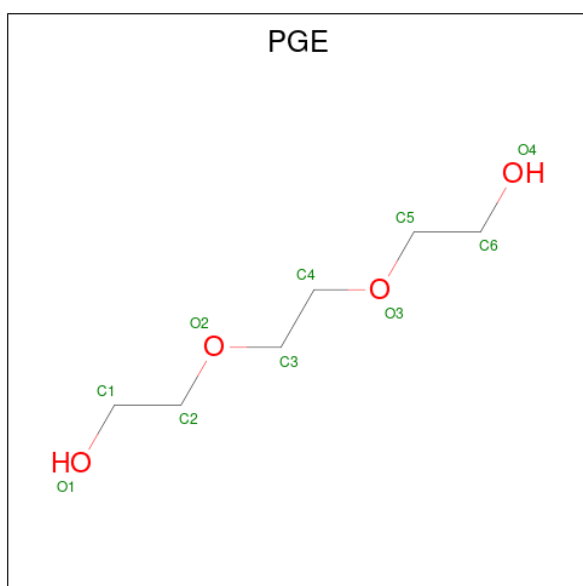
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	1
			12	6	6		
2	A	1	Total	C	O	0	0
			6	3	3		

- 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: $C_8H_{18}O_5$).

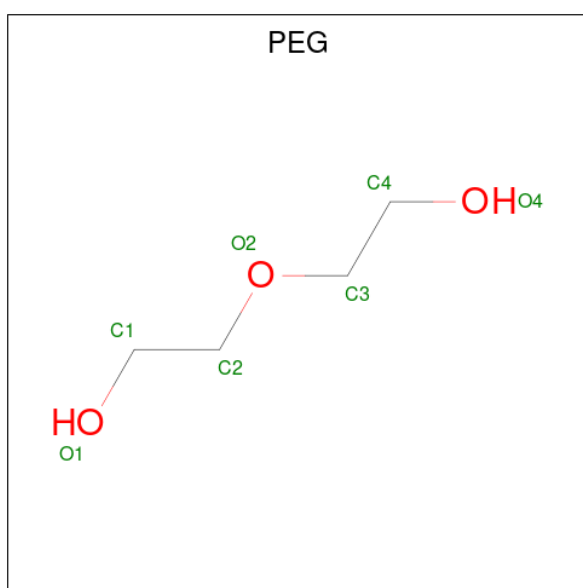


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- 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).

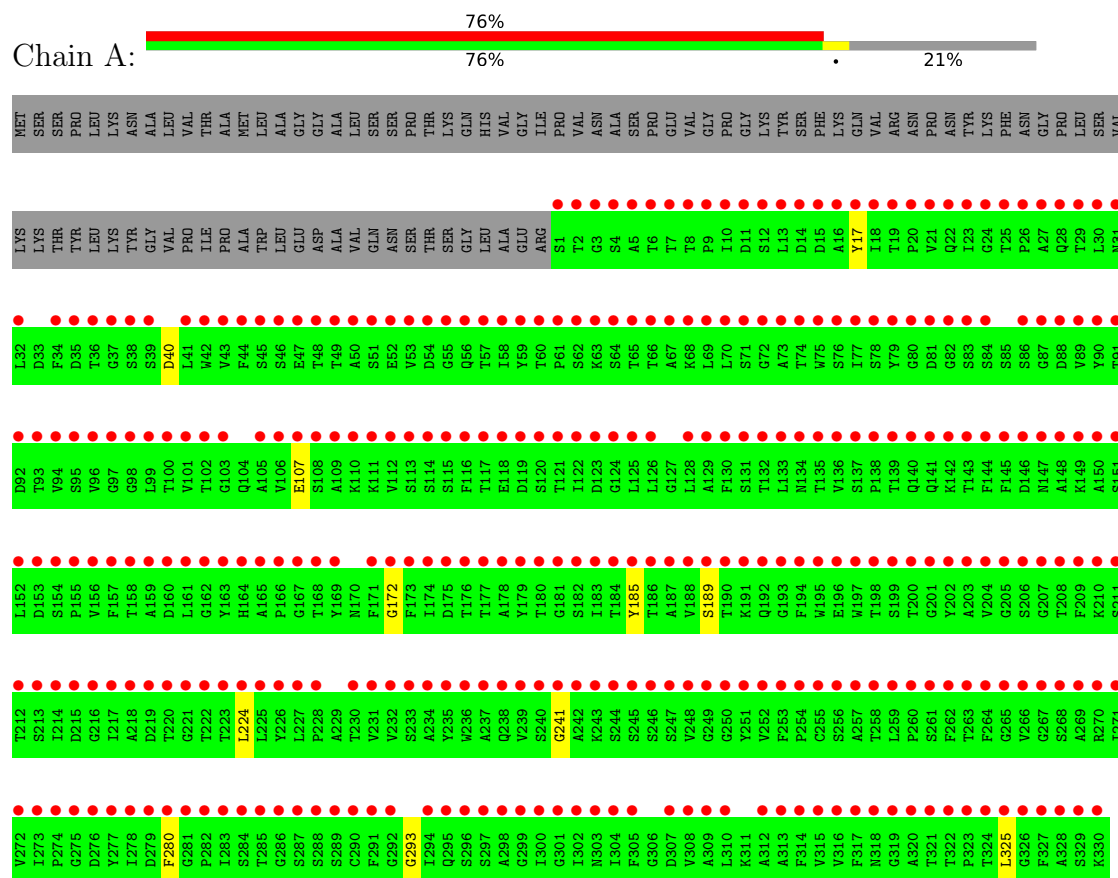


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.30Å 72.87Å 52.69Å 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) 89.4 (49.71-1.09)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.09Å)	Xtriage
Refinement program	REFMAC 5.8.0238, PHENIX 1.16.3549	Depositor
R, R_{free}	0.339 , 0.339 0.342 , 0.349	Depositor DCC
R_{free} test set	5792 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 14.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	2525	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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, PG4, ACT, GOL, PEG, NA

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	1.08	2/2552 (0.1%)	1.20	1/3496 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	SER	CA-CB	-5.38	1.45	1.53
1	A	17	TYR	C-O	5.33	1.30	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	PHE	CA-CB-CG	-6.26	107.53	113.80

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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%)	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. 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 oligosaccharides 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	$\# Z > 2$
4	PGE	A	406[A]	-	9,9,9	0.14	0	8,8,8	0.18	0
2	GOL	A	402[B]	-	5,5,5	0.11	0	5,5,5	0.28	0
2	GOL	A	403	-	5,5,5	0.06	0	5,5,5	0.20	0
3	ACT	A	405	-	3,3,3	1.14	0	3,3,3	0.72	0
2	GOL	A	401	-	5,5,5	0.12	0	5,5,5	0.43	0
7	PEG	A	409	-	6,6,6	0.14	0	5,5,5	0.09	0
2	GOL	A	402[A]	-	5,5,5	0.08	0	5,5,5	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	A	404[A]	-	3,3,3	0.92	0	3,3,3	0.86	0
5	PG4	A	407	6	12,12,12	0.16	0	11,11,11	0.13	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
4	PGE	A	406[A]	-	-	1/7/7/7	-
2	GOL	A	402[B]	-	-	2/4/4/4	-
2	GOL	A	403	-	-	2/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
7	PEG	A	409	-	-	1/4/4/4	-
2	GOL	A	402[A]	-	-	0/4/4/4	-
5	PG4	A	407	6	-	1/10/10/10	-

There are no bond length outliers.

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

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, 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%)	5.25	320 (96%) 0 0	5, 13, 20, 28	19 (5%)

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299[A]	GLY	13.9
1	A	197	TRP	12.7
1	A	300[A]	ILE	12.5
1	A	323	PRO	12.4
1	A	248	VAL	12.3
1	A	174[A]	ILE	12.0
1	A	321	THR	11.5
1	A	173	PHE	10.9
1	A	176	THR	10.8
1	A	53	VAL	10.4
1	A	150	ALA	10.2
1	A	208	THR	9.8
1	A	58	ILE	9.8
1	A	80	GLY	9.6
1	A	49	THR	9.3
1	A	232	VAL	9.3
1	A	180	THR	9.1
1	A	285	THR	9.1
1	A	236	TRP	8.9
1	A	249	GLY	8.9
1	A	130	PHE	8.9
1	A	166	PRO	8.9
1	A	283	ILE	8.9
1	A	54	ASP	8.8
1	A	319	GLY	8.7
1	A	198	THR	8.6
1	A	247	SER	8.5

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Mol	Chain	Res	Type	RSRZ
1	A	322	THR	8.5
1	A	133	LEU	8.5
1	A	320	ALA	8.4
1	A	212	THR	8.2
1	A	96	VAL	8.2
1	A	214	ILE	8.2
1	A	50	ALA	8.2
1	A	204	VAL	8.2
1	A	82	GLY	8.1
1	A	177	THR	8.0
1	A	16	ALA	8.0
1	A	51	SER	7.8
1	A	69	LEU	7.7
1	A	9[A]	PRO	7.7
1	A	111	LYS	7.7
1	A	151	SER	7.6
1	A	188	VAL	7.6
1	A	20	PRO	7.6
1	A	171	PHE	7.6
1	A	75	TRP	7.5
1	A	242	ALA	7.5
1	A	2	THR	7.4
1	A	48	THR	7.3
1	A	4	SER	7.3
1	A	71[A]	SER	7.3
1	A	81	ASP	7.2
1	A	302	ILE	7.2
1	A	13	LEU	7.1
1	A	209	PHE	7.1
1	A	258	THR	7.1
1	A	73	ALA	7.1
1	A	207	GLY	7.1
1	A	250	GLY	7.1
1	A	21	VAL	7.0
1	A	246[A]	SER	7.0
1	A	136	VAL	7.0
1	A	74	THR	7.0
1	A	70	LEU	6.9
1	A	251	TYR	6.9
1	A	44	PHE	6.9
1	A	184	THR	6.9
1	A	273	ILE	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	241	GLY	6.9
1	A	280	PHE	6.8
1	A	163	TYR	6.8
1	A	138	PRO	6.8
1	A	139	THR	6.8
1	A	79	TYR	6.7
1	A	195	TRP	6.7
1	A	90	TYR	6.6
1	A	105	ALA	6.6
1	A	94	VAL	6.6
1	A	253	PHE	6.6
1	A	112	VAL	6.5
1	A	26	PRO	6.5
1	A	78	SER	6.5
1	A	109	ALA	6.5
1	A	62	SER	6.4
1	A	259	LEU	6.4
1	A	55	GLY	6.4
1	A	77	ILE	6.4
1	A	117	THR	6.4
1	A	324	THR	6.4
1	A	310	LEU	6.3
1	A	66	THR	6.3
1	A	121	THR	6.3
1	A	143	THR	6.2
1	A	325[A]	LEU	6.2
1	A	149[A]	LYS	6.2
1	A	329	SER	6.2
1	A	262	PHE	6.2
1	A	93	THR	6.1
1	A	101	VAL	6.1
1	A	106	VAL	6.1
1	A	102	THR	6.1
1	A	59	TYR	6.1
1	A	65	THR	6.1
1	A	116	PHE	6.1
1	A	41	LEU	6.1
1	A	152	LEU	6.1
1	A	272	VAL	6.0
1	A	114	SER	5.9
1	A	61	PRO	5.9
1	A	17	TYR	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	316	VAL	5.8
1	A	98	GLY	5.8
1	A	99	LEU	5.8
1	A	122	ILE	5.8
1	A	228	PRO	5.8
1	A	25	THR	5.7
1	A	190	THR	5.7
1	A	110	LYS	5.7
1	A	308	VAL	5.7
1	A	23	ILE	5.7
1	A	215[A]	ASP	5.7
1	A	257	ALA	5.7
1	A	125	LEU	5.7
1	A	225	LEU	5.7
1	A	11	ASP	5.7
1	A	42	TRP	5.7
1	A	192	GLN	5.7
1	A	222	THR	5.6
1	A	290	CYS	5.6
1	A	57	THR	5.6
1	A	271	ILE	5.6
1	A	213	SER	5.6
1	A	67	ALA	5.5
1	A	186	THR	5.5
1	A	175	ASP	5.5
1	A	255	CYS	5.5
1	A	301	GLY	5.5
1	A	252	VAL	5.5
1	A	227	LEU	5.5
1	A	183	ILE	5.4
1	A	264	PHE	5.4
1	A	118	GLU	5.3
1	A	185	TYR	5.3
1	A	18	ILE	5.3
1	A	312	ALA	5.3
1	A	60	THR	5.3
1	A	146	ASP	5.3
1	A	291	PHE	5.3
1	A	286	GLY	5.3
1	A	318	ASN	5.3
1	A	202	TYR	5.2
1	A	145	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	194	PHE	5.2
1	A	8	THR	5.2
1	A	164	HIS	5.1
1	A	144	PHE	5.0
1	A	12	SER	5.0
1	A	156	VAL	5.0
1	A	275	GLY	5.0
1	A	178	ALA	5.0
1	A	153	ASP	5.0
1	A	113	SER	5.0
1	A	161	LEU	5.0
1	A	191	LYS	5.0
1	A	30	LEU	5.0
1	A	63	LYS	4.9
1	A	244	SER	4.9
1	A	27	ALA	4.9
1	A	72	GLY	4.9
1	A	115	SER	4.9
1	A	169	TYR	4.9
1	A	157	PHE	4.9
1	A	234	ALA	4.9
1	A	95	SER	4.9
1	A	172	GLY	4.8
1	A	245	SER	4.8
1	A	159	ALA	4.8
1	A	137	SER	4.8
1	A	327	PHE	4.8
1	A	206[A]	SER	4.8
1	A	179	TYR	4.7
1	A	199	SER	4.7
1	A	34	PHE	4.7
1	A	10	ILE	4.7
1	A	256	SER	4.6
1	A	165	ALA	4.6
1	A	254	PRO	4.6
1	A	120	SER	4.6
1	A	305	PHE	4.5
1	A	131	SER	4.5
1	A	167	GLY	4.5
1	A	132	THR	4.5
1	A	269	ALA	4.5
1	A	5	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	298[A]	ALA	4.4
1	A	328	ALA	4.4
1	A	304	ILE	4.4
1	A	201	GLY	4.4
1	A	211	SER	4.4
1	A	52	GLU	4.4
1	A	128	LEU	4.4
1	A	91	THR	4.4
1	A	200	THR	4.4
1	A	108	SER	4.3
1	A	68[A]	LYS	4.3
1	A	224	LEU	4.3
1	A	64	SER	4.3
1	A	277	TYR	4.3
1	A	158	THR	4.2
1	A	313	ALA	4.2
1	A	239	VAL	4.2
1	A	315	VAL	4.2
1	A	100	THR	4.2
1	A	314	PHE	4.2
1	A	38	SER	4.2
1	A	268[A]	SER	4.2
1	A	119	ASP	4.2
1	A	263	THR	4.2
1	A	217	ILE	4.1
1	A	226	TYR	4.1
1	A	43	VAL	4.1
1	A	76	SER	4.1
1	A	330	LYS	4.1
1	A	6	THR	4.1
1	A	260	PRO	4.1
1	A	220	THR	4.0
1	A	282	PRO	4.0
1	A	129	ALA	4.0
1	A	124	GLY	4.0
1	A	284	SER	4.0
1	A	187	ALA	4.0
1	A	168	THR	4.0
1	A	266	VAL	3.9
1	A	182[A]	SER	3.9
1	A	36	THR	3.9
1	A	274	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	288	SER	3.9
1	A	294	ILE	3.9
1	A	181	GLY	3.9
1	A	276[A]	ASP	3.9
1	A	148	ALA	3.9
1	A	7	THR	3.9
1	A	31	ASN	3.7
1	A	15	ASP	3.7
1	A	243	LYS	3.7
1	A	233	SER	3.7
1	A	265	GLY	3.7
1	A	203	ALA	3.7
1	A	83	SER	3.7
1	A	154[A]	SER	3.7
1	A	1	SER	3.6
1	A	231	VAL	3.6
1	A	140	GLN	3.6
1	A	235	TYR	3.6
1	A	289[A]	SER	3.6
1	A	142	LYS	3.5
1	A	29	THR	3.5
1	A	230	THR	3.5
1	A	162	GLY	3.5
1	A	155	PRO	3.5
1	A	240[A]	SER	3.4
1	A	88	ASP	3.4
1	A	134	ASN	3.4
1	A	3	GLY	3.4
1	A	28	GLN	3.3
1	A	278	ILE	3.2
1	A	135	THR	3.2
1	A	86	SER	3.2
1	A	297	SER	3.2
1	A	270	ARG	3.2
1	A	326	GLY	3.2
1	A	103	GLY	3.2
1	A	205	GLY	3.2
1	A	238	GLN	3.1
1	A	46	SER	3.1
1	A	237	ALA	3.1
1	A	309	ALA	3.1
1	A	223	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	317	PHE	3.0
1	A	35	ASP	2.9
1	A	39	SER	2.9
1	A	87	GLY	2.9
1	A	147	ASN	2.9
1	A	14	ASP	2.9
1	A	196	GLU	2.9
1	A	279	ASP	2.9
1	A	47	GLU	2.8
1	A	84	SER	2.8
1	A	32	LEU	2.7
1	A	37	GLY	2.7
1	A	189	SER	2.7
1	A	221	GLY	2.6
1	A	218	ALA	2.6
1	A	97	GLY	2.6
1	A	19	THR	2.6
1	A	193	GLY	2.6
1	A	292	GLY	2.5
1	A	261	SER	2.5
1	A	210	LYS	2.5
1	A	296	SER	2.5
1	A	92	ASP	2.5
1	A	45	SER	2.5
1	A	126	LEU	2.5
1	A	89	VAL	2.4
1	A	56	GLN	2.4
1	A	303	ASN	2.4
1	A	219	ASP	2.4
1	A	216	GLY	2.4
1	A	267	GLY	2.4
1	A	141	GLN	2.4
1	A	22	GLN	2.3
1	A	107	GLU	2.2
1	A	287	SER	2.2
1	A	160	ASP	2.2
1	A	307	ASP	2.2
1	A	295	GLN	2.1
1	A	281	GLY	2.1
1	A	123	ASP	2.0
1	A	24	GLY	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($\text{\AA}^2$)	Q<0.9
7	PEG	A	409	7/7	0.30	0.63	53,55,56,56	0
3	ACT	A	404[A]	4/4	0.41	0.60	21,22,23,23	4
2	GOL	A	403	6/6	0.44	0.51	25,30,31,31	6
4	PGE	A	406[A]	10/10	0.51	0.49	32,33,35,35	10
2	GOL	A	402[A]	6/6	0.52	0.36	18,20,21,21	6
2	GOL	A	402[B]	6/6	0.52	0.36	18,23,23,25	6
5	PG4	A	407	13/13	0.56	0.40	36,37,39,39	0
6	NA	A	408	1/1	0.57	0.47	56,56,56,56	0
3	ACT	A	405	4/4	0.63	0.29	25,26,27,28	0
2	GOL	A	401	6/6	0.81	0.25	14,17,19,22	6

6.5 Other polymers [i](#)

There are no such residues in this entry.