



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:21 PM UTC

PDB ID : 9SPA / pdb_00009spa
Title : Apo ACE2 extracellular domain
Authors : Brear, P.; Hyvonen, M.
Deposited on : 2025-09-16
Resolution : 1.79 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

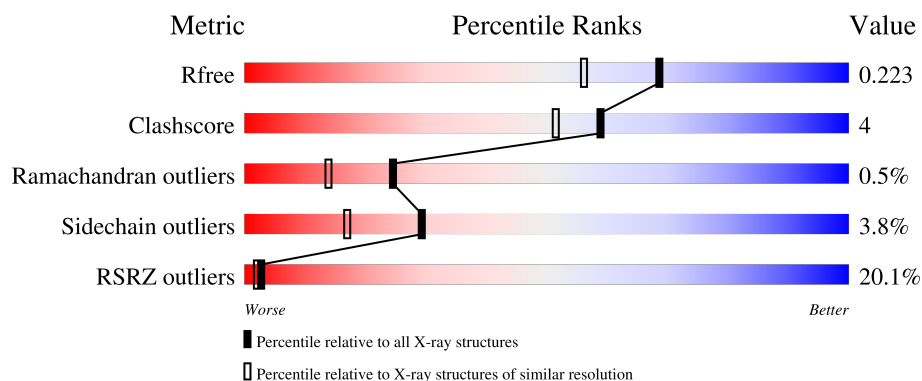
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	C	609	<div> <div>20%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5310 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.

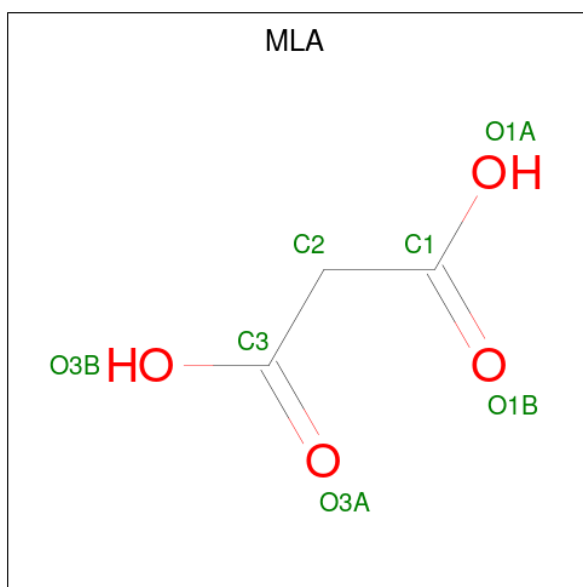
- Molecule 1 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	596	4882	3121	809	923	29	0	3	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP Q9BYF1
C	598	SER	-	expression tag	UNP Q9BYF1
C	599	SER	-	expression tag	UNP Q9BYF1
C	600	PRO	-	expression tag	UNP Q9BYF1
C	601	HIS	-	expression tag	UNP Q9BYF1
C	602	HIS	-	expression tag	UNP Q9BYF1
C	603	HIS	-	expression tag	UNP Q9BYF1
C	604	HIS	-	expression tag	UNP Q9BYF1
C	605	HIS	-	expression tag	UNP Q9BYF1
C	606	HIS	-	expression tag	UNP Q9BYF1
C	607	HIS	-	expression tag	UNP Q9BYF1
C	608	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is MALONIC ACID (CCD ID: MLA) (formula: C₃H₄O₄).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Zn	0	0
			1	1		

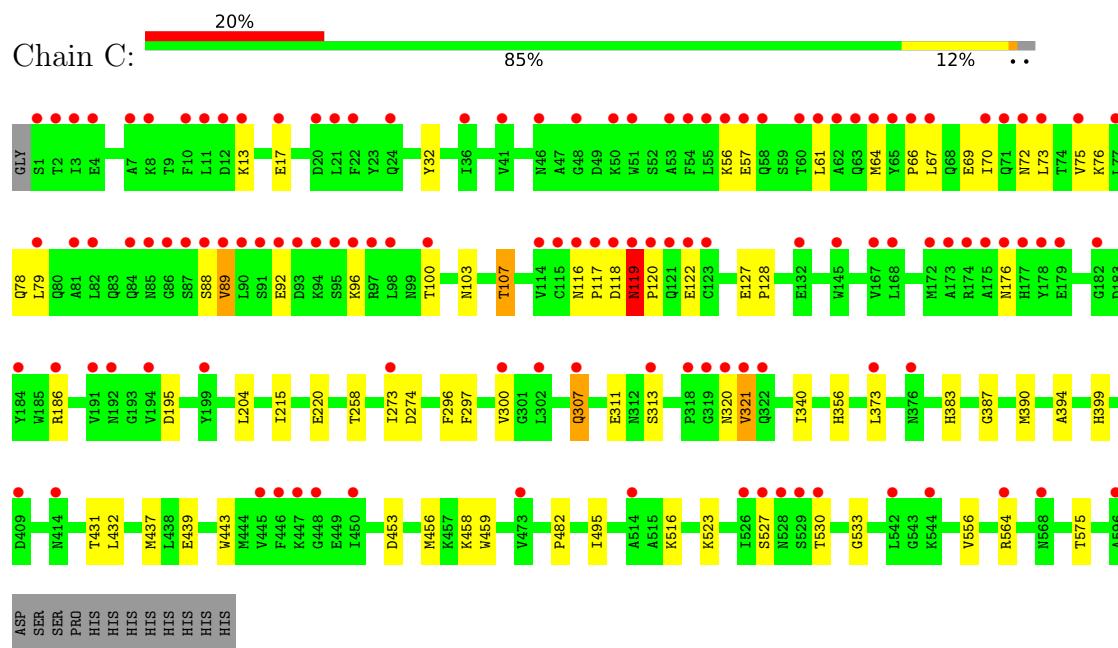
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	419	Total	O	0	1
			420	420		

3 Residue-property plots [i](#)

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: Processed angiotensin-converting enzyme 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	163.35Å 163.35Å 71.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.50 – 1.79 115.50 – 1.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (115.50-1.79) 100.0 (115.50-1.79)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.78Å)	Xtriage
Refinement program	BUSTER 2.10.4 (10-JUL-2024)	Depositor
R, R_{free}	0.221 , 0.238 0.215 , 0.223	Depositor DCC
R_{free} test set	1998 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5310	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: ZN, MLA

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	C	0.80	0/5019	1.04	2/6819 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	453	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	274	ASP	N-CA-C	-5.42	99.68	108.41

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	C	4882	0	4655	42	0
2	C	7	0	2	0	0
3	C	1	0	0	0	0
4	C	420	0	0	1	0
All	All	5310	0	4657	42	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 4.

All (42) 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:C:61:LEU:HA	1:C:64:MET:HE3	1.47	0.94
1:C:72:ASN:HB3	1:C:75:VAL:HG22	1.67	0.77
1:C:118:ASP:O	1:C:119:ASN:HB2	1.93	0.68
1:C:72:ASN:HD22	1:C:75:VAL:HG13	1.58	0.67
1:C:32:TYR:OH	1:C:107:THR:HG22	1.99	0.63
1:C:103:ASN:O	1:C:107:THR:HG23	2.04	0.58
1:C:186:ARG:HG2	1:C:204:LEU:HD23	1.85	0.58
1:C:119:ASN:HB3	1:C:122:GLU:HB2	1.88	0.56
1:C:300:VAL:O	1:C:533:GLY:HA3	2.07	0.55
1:C:297:PHE:O	1:C:300:VAL:HG22	2.07	0.54
1:C:70:ILE:HG21	1:C:75:VAL:HG23	1.88	0.53
1:C:320:ASN:O	1:C:321:VAL:HB	2.09	0.53
1:C:72:ASN:ND2	1:C:75:VAL:HG13	2.22	0.53
1:C:307:GLN:OE1	1:C:311:GLU:OE1	2.26	0.53
1:C:67:LEU:HB3	1:C:76:LYS:NZ	2.24	0.52
1:C:70:ILE:CG2	1:C:75:VAL:HG23	2.40	0.52
1:C:57:GLU:O	1:C:61:LEU:HG	2.10	0.51
1:C:72:ASN:HB3	1:C:75:VAL:CG2	2.40	0.50
1:C:215:ILE:HD13	1:C:432:LEU:HD13	1.93	0.49
1:C:116:ASN:O	1:C:117:PRO:C	2.55	0.48
1:C:13:LYS:HE2	1:C:17:GLU:OE2	2.14	0.48
1:C:297:PHE:CE1	1:C:390:MET:HG3	2.48	0.48
1:C:96:LYS:O	1:C:100:THR:HG23	2.14	0.47
1:C:66:PRO:CG	1:C:69:GLU:HG3	2.45	0.47
1:C:459:TRP:CE3	1:C:482:PRO:HG3	2.50	0.46
1:C:394:ALA:HA	1:C:399:HIS:CD2	2.50	0.46
1:C:313:SER:HB2	1:C:340:ILE:O	2.16	0.45
1:C:439:GLU:HG2	1:C:495:ILE:HB	2.01	0.43
1:C:220:GLU:HG3	4:C:1084:HOH:O	2.17	0.43
1:C:119:ASN:H	1:C:120:PRO:HD3	1.84	0.42
1:C:88:SER:HB2	1:C:176:ASN:OD1	2.19	0.42
1:C:72:ASN:HD22	1:C:75:VAL:H	1.66	0.42
1:C:66:PRO:HG2	1:C:69:GLU:HB2	2.01	0.42
1:C:127:GLU:HA	1:C:128:PRO:HA	1.87	0.42
1:C:300:VAL:HG21	1:C:390:MET:HE1	2.00	0.42
1:C:456:MET:HE1	1:C:482:PRO:CD	2.50	0.41
1:C:356:HIS:HA	1:C:387:GLY:HA3	2.01	0.41
1:C:78:GLN:HB3	1:C:373:LEU:HD12	2.02	0.41
1:C:186:ARG:HH11	1:C:443:TRP:CG	2.39	0.41
1:C:296:PHE:HE1	1:C:527:SER:OG	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:SER:O	1:C:89:VAL:HB	2.21	0.41
1:C:296:PHE:CE1	1:C:527:SER:OG	2.74	0.40

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	C	597/609 (98%)	579 (97%)	15 (2%)	3 (0%)	24 14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	VAL
1	C	119	ASN
1	C	321	VAL

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	C	529/538 (98%)	509 (96%)	20 (4%)	29 17

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	56	LYS
1	C	73	LEU
1	C	79	LEU
1	C	92	GLU
1	C	107	THR
1	C	119	ASN
1	C	195	ASP
1	C	258	THR
1	C	273	ILE
1	C	307	GLN
1	C	383	HIS
1	C	431	THR
1	C	437	MET
1	C	458	LYS
1	C	516	LYS
1	C	523	LYS
1	C	530	THR
1	C	556	VAL
1	C	564	ARG
1	C	575	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	31	ASN
1	C	35	ASN
1	C	40	ASN
1	C	58	GLN
1	C	63	GLN
1	C	72	ASN
1	C	78	GLN
1	C	119	ASN
1	C	131	ASN
1	C	312	ASN
1	C	322	GLN
1	C	454	GLN
1	C	490	ASN
1	C	517	HIS

5.3.3 RNA ⓘ

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	MLA	C	701	3	6,6,6	1.27	0	7,7,7	1.12	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	MLA	C	701	3	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	MLA	O1A-C1-C2-C3
2	C	701	MLA	O1B-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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	C	596/609 (97%)	1.02	120 (20%) 3 2	19, 38, 73, 90	3 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	596	ALA	8.3
1	C	321	VAL	7.5
1	C	90	LEU	6.6
1	C	3	ILE	5.7
1	C	85	ASN	5.6
1	C	120	PRO	5.0
1	C	87	SER	5.0
1	C	300	VAL	4.9
1	C	61	LEU	4.8
1	C	2	THR	4.7
1	C	91	SER	4.6
1	C	117	PRO	4.5
1	C	89	VAL	4.5
1	C	70	ILE	4.4
1	C	64	MET	4.3
1	C	86	GLY	4.3
1	C	65	TYR	4.1
1	C	116	ASN	4.0
1	C	320	ASN	4.0
1	C	79	LEU	3.8
1	C	184	TYR	3.8
1	C	175	ALA	3.7
1	C	194	VAL	3.7
1	C	67	LEU	3.7
1	C	121	GLN	3.7
1	C	174	ARG	3.6
1	C	118	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	62	ALA	3.6
1	C	88	SER	3.6
1	C	177	HIS	3.5
1	C	528	ASN	3.4
1	C	73	LEU	3.4
1	C	82	LEU	3.4
1	C	273	ILE	3.3
1	C	191	VAL	3.3
1	C	122	GLU	3.2
1	C	94	LYS	3.2
1	C	529	SER	3.2
1	C	568[A]	ASN	3.2
1	C	448	GLY	3.2
1	C	17	GLU	3.2
1	C	98	LEU	3.1
1	C	176	ASN	3.1
1	C	95	SER	3.1
1	C	66	PRO	3.1
1	C	172	MET	3.0
1	C	313	SER	3.0
1	C	526	ILE	3.0
1	C	1	SER	2.9
1	C	115	CYS	2.9
1	C	173	ALA	2.9
1	C	10	PHE	2.8
1	C	41	VAL	2.8
1	C	75	VAL	2.8
1	C	7	ALA	2.8
1	C	409	ASP	2.8
1	C	100	THR	2.8
1	C	527	SER	2.8
1	C	77	LEU	2.7
1	C	178	TYR	2.7
1	C	81	ALA	2.7
1	C	55	LEU	2.7
1	C	530	THR	2.7
1	C	92	GLU	2.6
1	C	84	GLN	2.6
1	C	307	GLN	2.6
1	C	192	ASN	2.6
1	C	376	ASN	2.6
1	C	544	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	445	VAL	2.6
1	C	72	ASN	2.6
1	C	60	THR	2.5
1	C	8	LYS	2.5
1	C	13	LYS	2.5
1	C	20	ASP	2.5
1	C	22	PHE	2.5
1	C	93	ASP	2.5
1	C	167	VAL	2.5
1	C	96	LYS	2.4
1	C	319	GLY	2.4
1	C	4	GLU	2.4
1	C	50	LYS	2.4
1	C	24	GLN	2.4
1	C	318	PRO	2.4
1	C	11	LEU	2.4
1	C	564	ARG	2.4
1	C	119	ASN	2.3
1	C	123	CYS	2.3
1	C	168	LEU	2.3
1	C	51	TRP	2.3
1	C	473	VAL	2.3
1	C	302	LEU	2.3
1	C	54	PHE	2.3
1	C	186	ARG	2.3
1	C	46	ASN	2.3
1	C	56	LYS	2.3
1	C	450	ILE	2.3
1	C	114	VAL	2.3
1	C	58	GLN	2.2
1	C	179	GLU	2.2
1	C	199	TYR	2.2
1	C	145	TRP	2.2
1	C	514	ALA	2.2
1	C	36	ILE	2.2
1	C	97	ARG	2.2
1	C	373	LEU	2.2
1	C	542	LEU	2.2
1	C	446	PHE	2.2
1	C	447	LYS	2.2
1	C	12	ASP	2.1
1	C	71	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	322	GLN	2.1
1	C	53	ALA	2.1
1	C	21	LEU	2.1
1	C	57	GLU	2.1
1	C	132	GLU	2.1
1	C	414	ASN	2.1
1	C	63	GLN	2.1
1	C	48	GLY	2.0
1	C	182	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(Å ²)	Q<0.9
2	MLA	C	701	7/7	0.97	0.06	31,32,35,36	0
3	ZN	C	702	1/1	0.99	0.04	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.