



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:33 AM UTC

PDB ID : 4EE2 / pdb_00004ee2
Title : Crystal Structure of Anthrax Protective Antigen K446M Mutant to 1.91-A
Resolution
Authors : Kintzer, A.F.; Krantz, B.A.
Deposited on : 2012-03-28
Resolution : 1.91 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
Xtrriage (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

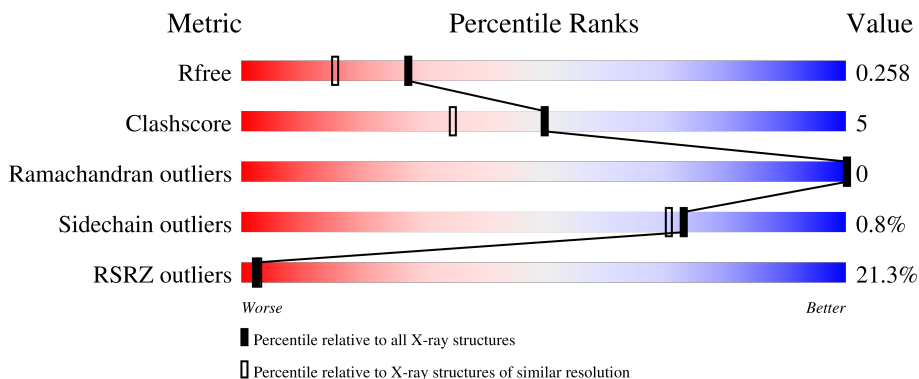
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	736	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5709 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 Protective antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	701	5560	3474	955	1122	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P13423
A	446	MET	LYS	engineered mutation	UNP P13423

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

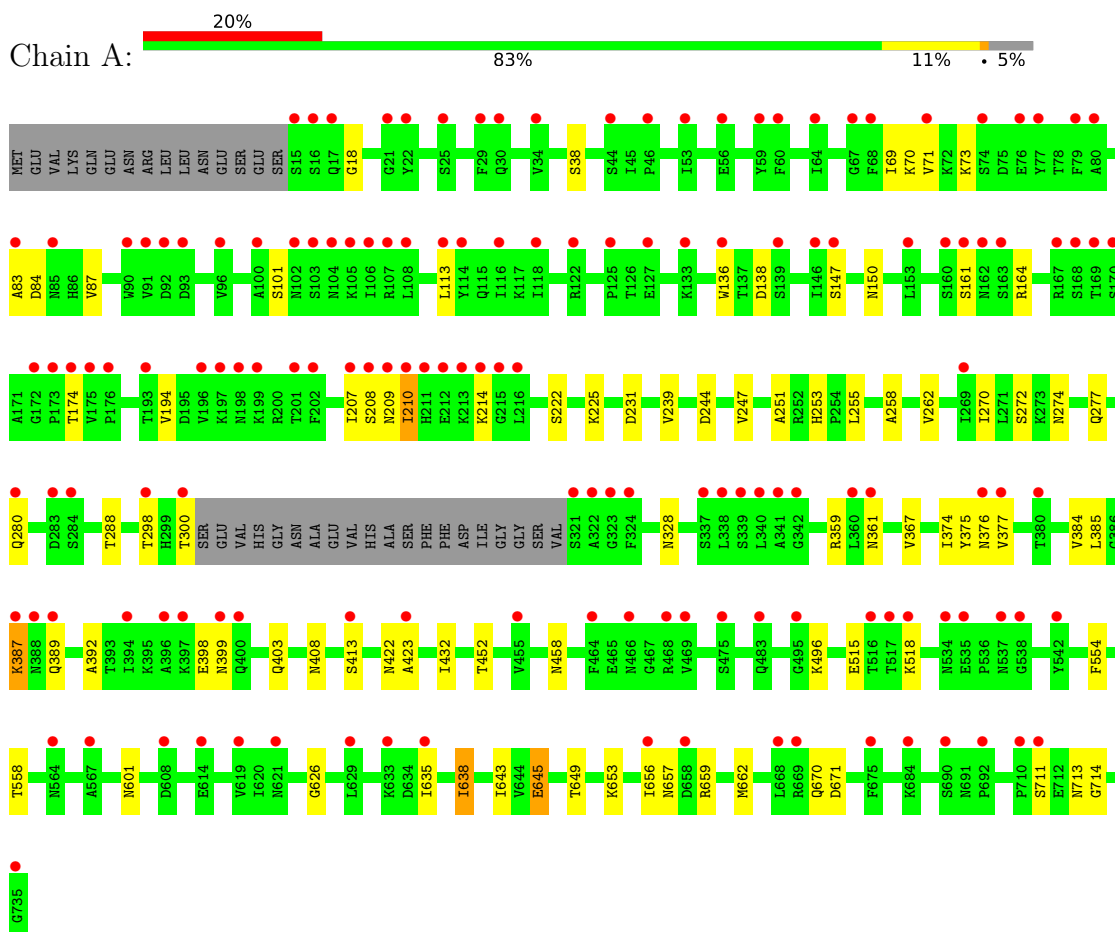
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total	O	0	0
			147	147		

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: Protective antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.22Å 93.51Å 116.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.69 – 1.91 40.69 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.69-1.91) 93.0 (40.69-1.91)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.91Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.229 , 0.265 0.227 , 0.258	Depositor DCC
R_{free} test set	2000 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtrriage
Anisotropy	0.700	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5709	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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:
CA

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	0.45	0/5658	0.80	9/7668 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	SER	N-CA-C	7.91	119.53	111.07
1	A	210	ILE	N-CA-C	7.90	119.61	111.00
1	A	375	TYR	N-CA-C	5.78	120.37	112.68
1	A	387	LYS	N-CA-C	5.65	117.52	111.36
1	A	656	ILE	N-CA-C	5.65	115.84	110.42
1	A	713	ASN	N-CA-C	-5.43	105.75	112.38
1	A	231	ASP	CA-C-N	-5.39	114.75	121.00
1	A	231	ASP	C-N-CA	-5.39	114.75	121.00
1	A	626	GLY	N-CA-C	5.35	118.28	110.63

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	5560	0	5476	58	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	147	0	0	4	0
All	All	5709	0	5476	58	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 5.

All (58) 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:384:VAL:HG13	1:A:389:GLN:O	1.51	1.11
1:A:253:HIS:HD2	1:A:255:LEU:H	1.18	0.88
1:A:272:SER:HB3	1:A:288:THR:HG22	1.55	0.86
1:A:403:GLN:HE22	1:A:413:SER:H	1.34	0.76
1:A:385:LEU:O	1:A:389:GLN:HB2	1.88	0.73
1:A:384:VAL:CG1	1:A:389:GLN:O	2.39	0.61
1:A:194:VAL:HG21	1:A:239:VAL:HB	1.83	0.59
1:A:374:ILE:HG21	1:A:377:VAL:O	2.04	0.58
1:A:147:SER:OG	1:A:150:ASN:ND2	2.38	0.56
1:A:84:ASP:OD2	1:A:101:SER:HA	2.04	0.56
1:A:253:HIS:CD2	1:A:255:LEU:H	2.10	0.56
1:A:69:ILE:HD11	1:A:136:TRP:CZ3	2.42	0.55
1:A:161:SER:HB3	1:A:164:ARG:HB2	1.89	0.55
1:A:376:ASN:ND2	1:A:458:ASN:OD1	2.33	0.54
1:A:174:THR:O	1:A:174:THR:HG23	2.07	0.53
1:A:274:ASN:HD22	1:A:359:ARG:HH11	1.56	0.53
1:A:274:ASN:ND2	1:A:359:ARG:HH11	2.08	0.52
1:A:643:ILE:HA	1:A:657:ASN:HD21	1.75	0.51
1:A:253:HIS:HE1	3:A:990:HOH:O	1.91	0.51
1:A:635:ILE:O	1:A:638:ILE:HG13	2.10	0.51
1:A:422:ASN:OD1	3:A:1012:HOH:O	2.20	0.50
1:A:711:SER:O	1:A:714:GLY:N	2.44	0.50
1:A:671:ASP:OD1	1:A:671:ASP:N	2.44	0.50
1:A:398:GLU:O	1:A:399:ASN:HB2	2.11	0.49
1:A:83:ALA:O	1:A:87:VAL:HG23	2.13	0.49
1:A:277:GLN:O	1:A:280:GLN:NE2	2.46	0.49
1:A:515:GLU:OE1	1:A:518:LYS:HE2	2.12	0.48
1:A:222:SER:HB2	1:A:518:LYS:HG2	1.95	0.48
1:A:225:LYS:HD3	1:A:518:LYS:HD3	1.95	0.48
1:A:138:ASP:OD1	1:A:138:ASP:C	2.57	0.47
1:A:274:ASN:HD21	1:A:359:ARG:HB3	1.78	0.47
1:A:270:ILE:CG2	1:A:361:ASN:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLY:HA3	1:A:38:SER:O	2.15	0.46
1:A:422:ASN:HB2	3:A:1011:HOH:O	2.14	0.46
1:A:270:ILE:HG23	1:A:361:ASN:HB3	1.98	0.46
1:A:374:ILE:CG2	1:A:377:VAL:O	2.64	0.46
1:A:328:ASN:HB2	1:A:452:THR:O	2.16	0.45
1:A:210:ILE:O	1:A:214:LYS:HG2	2.18	0.44
1:A:392:ALA:HB2	1:A:432:ILE:HG23	2.00	0.44
1:A:515:GLU:OE1	1:A:518:LYS:NZ	2.50	0.43
1:A:659:ARG:HD3	1:A:662:MET:HE3	1.99	0.43
1:A:423:ALA:O	3:A:1012:HOH:O	2.21	0.43
1:A:70:LYS:HB3	1:A:113:LEU:HD23	2.01	0.43
1:A:209:ASN:OD1	1:A:210:ILE:N	2.51	0.43
1:A:408:ASN:HD21	1:A:496:LYS:NZ	2.16	0.42
1:A:645:GLU:CD	1:A:653:LYS:HD3	2.44	0.42
1:A:71:VAL:HG22	1:A:73:LYS:H	1.84	0.42
1:A:403:GLN:NE2	1:A:413:SER:H	2.10	0.42
1:A:174:THR:O	1:A:174:THR:CG2	2.68	0.42
1:A:207:ILE:HG22	1:A:209:ASN:OD1	2.20	0.41
1:A:244:ASP:HB3	1:A:247:VAL:HG23	2.03	0.41
1:A:251:ALA:HB1	1:A:258:ALA:HB2	2.01	0.41
1:A:225:LYS:CD	1:A:518:LYS:HD3	2.50	0.41
1:A:298:THR:HB	1:A:601:ASN:HB3	2.02	0.41
1:A:387:LYS:HB2	1:A:387:LYS:HE2	1.74	0.41
1:A:262:VAL:HA	1:A:367:VAL:O	2.21	0.41
1:A:515:GLU:OE1	1:A:518:LYS:CE	2.69	0.41
1:A:554:PHE:HB3	1:A:558:THR:HB	2.04	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	A	697/736 (95%)	685 (98%)	12 (2%)	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	630/662 (95%)	625 (99%)	5 (1%)	73	71

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	THR
1	A	638	ILE
1	A	645	GLU
1	A	649	THR
1	A	670	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	86	HIS
1	A	150	ASN
1	A	158	GLN
1	A	180	ASN
1	A	246	ASN
1	A	253	HIS
1	A	274	ASN
1	A	280	GLN
1	A	400	GLN
1	A	403	GLN
1	A	408	ASN
1	A	437	ASN

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Mol	Chain	Res	Type
1	A	534	ASN
1	A	541	GLN
1	A	560	GLN
1	A	584	ASN
1	A	601	ASN
1	A	670	GLN
1	A	705	ASN
1	A	709	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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	701/736 (95%)	1.36	149 (21%) 2 3	26, 41, 70, 90	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	SER	6.2
1	A	324	PHE	4.8
1	A	83	ALA	4.7
1	A	341	ALA	4.7
1	A	377	VAL	4.3
1	A	93	ASP	4.3
1	A	212	GLU	4.3
1	A	342	GLY	4.2
1	A	340	LEU	4.1
1	A	210	ILE	4.0
1	A	339	SER	4.0
1	A	175	VAL	4.0
1	A	176	PRO	4.0
1	A	516	THR	3.9
1	A	338	LEU	3.9
1	A	113	LEU	3.8
1	A	300	THR	3.6
1	A	169	THR	3.5
1	A	517	THR	3.5
1	A	102	ASN	3.5
1	A	711	SER	3.5
1	A	337	SER	3.4
1	A	71	VAL	3.4
1	A	658	ASP	3.4
1	A	91	VAL	3.3
1	A	196	VAL	3.3
1	A	322	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	15	SER	3.2
1	A	361	ASN	3.2
1	A	108	LEU	3.2
1	A	136	TRP	3.1
1	A	207	ILE	3.1
1	A	534	ASN	3.1
1	A	16	SER	3.1
1	A	80	ALA	3.1
1	A	216	LEU	3.1
1	A	197	LYS	3.1
1	A	633	LYS	3.1
1	A	79	PHE	3.1
1	A	105	LYS	3.0
1	A	389	GLN	3.0
1	A	17	GLN	3.0
1	A	538	GLY	3.0
1	A	25	SER	3.0
1	A	283	ASP	2.9
1	A	22	TYR	2.9
1	A	298	THR	2.9
1	A	468	ARG	2.9
1	A	174	THR	2.8
1	A	92	ASP	2.8
1	A	710	PRO	2.8
1	A	44	SER	2.8
1	A	376	ASN	2.7
1	A	34	VAL	2.7
1	A	67	GLY	2.7
1	A	735	GLY	2.7
1	A	629	LEU	2.7
1	A	163	SER	2.7
1	A	172	GLY	2.7
1	A	413	SER	2.7
1	A	537	ASN	2.7
1	A	323	GLY	2.6
1	A	56	GLU	2.6
1	A	475	SER	2.6
1	A	690	SER	2.6
1	A	360	LEU	2.6
1	A	53	ILE	2.6
1	A	684	LYS	2.6
1	A	388	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	394	ILE	2.6
1	A	198	ASN	2.6
1	A	173	PRO	2.6
1	A	74	SER	2.6
1	A	139	SER	2.6
1	A	30	GLN	2.5
1	A	387	LYS	2.5
1	A	518	LYS	2.5
1	A	321	SER	2.5
1	A	199	LYS	2.5
1	A	106	ILE	2.5
1	A	466	ASN	2.5
1	A	167	ARG	2.5
1	A	214	LYS	2.5
1	A	160	SER	2.5
1	A	635	ILE	2.5
1	A	400	GLN	2.5
1	A	193	THR	2.5
1	A	107	ARG	2.4
1	A	423	ALA	2.4
1	A	455	VAL	2.4
1	A	621	ASN	2.4
1	A	76	GLU	2.4
1	A	211	HIS	2.4
1	A	59	TYR	2.4
1	A	675	PHE	2.4
1	A	668	LEU	2.4
1	A	614	GLU	2.4
1	A	125	PRO	2.4
1	A	161	SER	2.4
1	A	170	SER	2.4
1	A	127	GLU	2.3
1	A	201	THR	2.3
1	A	146	ILE	2.3
1	A	21	GLY	2.3
1	A	495	GLY	2.3
1	A	168	SER	2.3
1	A	77	TYR	2.3
1	A	564	ASN	2.3
1	A	619	VAL	2.3
1	A	100	ALA	2.3
1	A	96	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	133	LYS	2.3
1	A	29	PHE	2.2
1	A	64	ILE	2.2
1	A	380	THR	2.2
1	A	114	TYR	2.2
1	A	118	ILE	2.2
1	A	269	ILE	2.2
1	A	656	ILE	2.2
1	A	535	GLU	2.2
1	A	60	PHE	2.2
1	A	202	PHE	2.2
1	A	213	LYS	2.2
1	A	669	ARG	2.2
1	A	122	ARG	2.2
1	A	68	PHE	2.1
1	A	85	ASN	2.1
1	A	162	ASN	2.1
1	A	209	ASN	2.1
1	A	464	PHE	2.1
1	A	90	TRP	2.1
1	A	280	GLN	2.1
1	A	608	ASP	2.1
1	A	284	SER	2.1
1	A	116	ILE	2.1
1	A	103	SER	2.1
1	A	215	GLY	2.1
1	A	483	GLN	2.1
1	A	567	ALA	2.1
1	A	399	ASN	2.1
1	A	153	LEU	2.1
1	A	396	ALA	2.1
1	A	397	LYS	2.0
1	A	542	TYR	2.0
1	A	46	PRO	2.0
1	A	469	VAL	2.0
1	A	147	SER	2.0
1	A	104	ASN	2.0
1	A	692	PRO	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	CA	A	800	1/1	0.95	0.06	29,29,29,29	0
2	CA	A	801	1/1	0.95	0.06	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.