



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:40 PM UTC

PDB ID : 1IKP / pdb_00001ikp
Title : Pseudomonas Aeruginosa Exotoxin A, P201Q, W281A mutant
Authors : McKay, D.B.; Wedekind, J.E.; Trame, C.B.
Deposited on : 2001-05-04
Resolution : 1.45 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
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

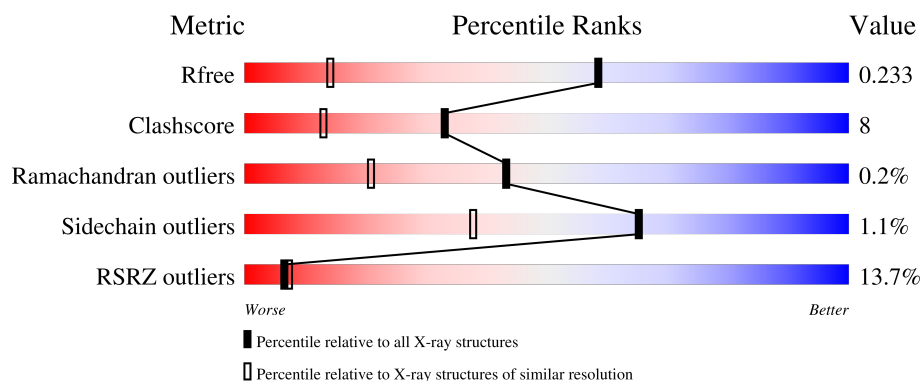
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	613	13% 82% 14% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5185 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 EXOTOXIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	599	Total	C	N	O	S	0	9	0
			4641	2898	837	892	14			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	GLN	PRO	engineered mutation	UNP P11439
A	281	ALA	TRP	engineered mutation	UNP P11439
A	364	ASN	SER	SEE REMARK 999	UNP P11439
A	407	VAL	ILE	SEE REMARK 999	UNP P11439
A	515	SER	GLY	SEE REMARK 999	UNP P11439

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		

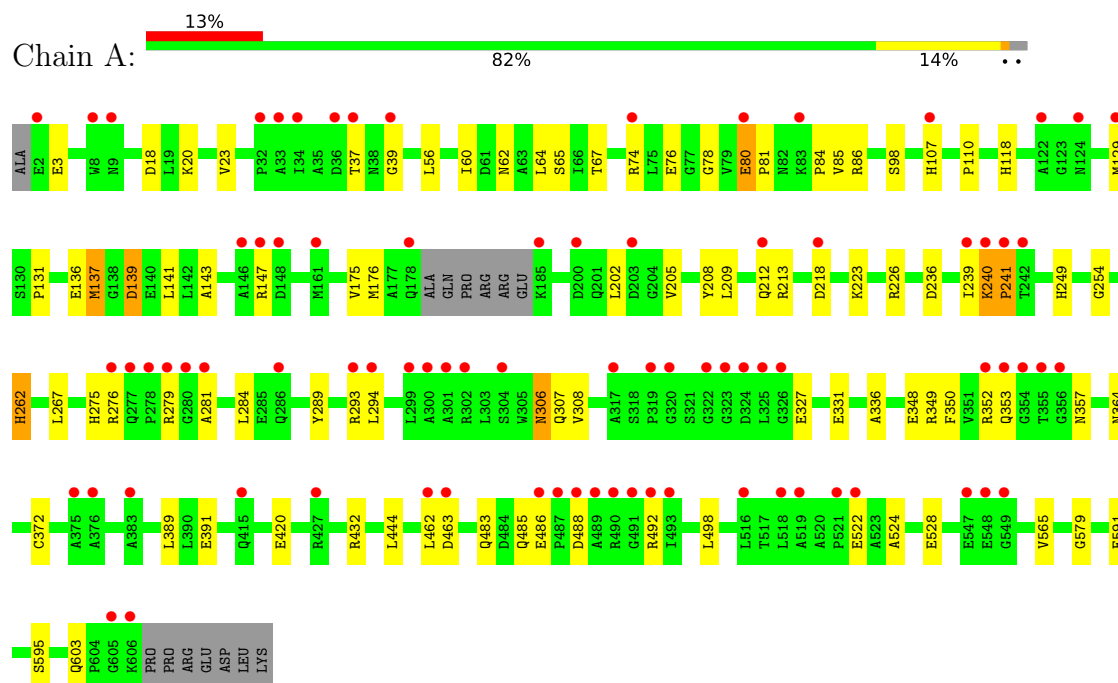
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	540	Total	O	0	0
			540	540		

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: EXOTOXIN A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.91Å 99.07Å 58.63Å 90.00° 97.34° 90.00°	Depositor
Resolution (Å)	21.82 – 1.45 21.82 – 1.45	Depositor EDS
% Data completeness (in resolution range)	90.2 (21.82-1.45) 90.2 (21.82-1.45)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 1.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.205 , 0.228 0.209 , 0.233	Depositor DCC
R_{free} test set	11675 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5185	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.50	1/4740 (0.0%)	0.93	19/6447 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	PRO	N-CD	5.38	1.55	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	PRO	N-CA-C	8.38	124.55	113.57
1	A	107	HIS	N-CA-C	6.59	118.46	111.28
1	A	389	LEU	N-CA-C	-6.32	100.21	110.20
1	A	372	CYS	N-CA-C	6.16	118.56	109.62
1	A	110	PRO	N-CA-C	-5.93	102.16	111.34
1	A	239	ILE	N-CA-C	5.85	117.62	109.55
1	A	56	LEU	N-CA-C	5.82	118.26	109.23
1	A	565	VAL	N-CA-C	-5.69	100.14	108.11
1	A	139	ASP	N-CA-C	5.59	117.05	111.07
1	A	218	ASP	N-CA-C	5.53	118.02	111.33
1	A	62	ASN	N-CA-C	-5.51	106.14	112.92
1	A	236	ASP	N-CA-C	-5.42	102.85	110.50
1	A	595	SER	N-CA-C	5.33	119.34	112.41
1	A	209	LEU	N-CA-C	5.21	117.04	111.36
1	A	131	PRO	N-CA-C	-5.13	103.72	111.41
1	A	240	LYS	CA-C-N	5.12	126.24	119.84
1	A	240	LYS	C-N-CA	5.12	126.24	119.84
1	A	591	GLU	N-CA-C	-5.11	105.79	111.36
1	A	444	LEU	N-CA-C	5.09	117.22	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4641	0	4506	71	0
2	A	2	0	0	0	0
3	A	2	0	0	0	0
4	A	540	0	0	10	0
All	All	5185	0	4506	71	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 8.

All (71) 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:37:THR:HG22	1:A:39:GLY:H	1.23	1.03
1:A:137:MET:HE2	1:A:141:LEU:HD23	1.39	0.99
1:A:137:MET:HE3	1:A:137:MET:HA	1.42	0.98
1:A:137:MET:HA	1:A:137:MET:CE	1.95	0.96
1:A:137:MET:CE	1:A:141:LEU:HD23	2.13	0.79
1:A:129:MET:HE1	1:A:205:VAL:HG11	1.69	0.74
1:A:348:GLU:HG2	1:A:352:ARG:HH11	1.54	0.72
1:A:262:HIS:HE1	1:A:391:GLU:OE2	1.74	0.71
1:A:348:GLU:HG2	1:A:352:ARG:NH1	2.06	0.70
1:A:212:GLN:HE22	1:A:432:ARG:HE	1.41	0.69
1:A:226:ARG:HD3	4:A:756:HOH:O	1.93	0.67
1:A:327:GLU:O	1:A:331:GLU:HG3	1.95	0.66
1:A:483:GLN:HE22	1:A:579:GLY:HA2	1.62	0.64
1:A:488:ASP:OD1	1:A:492:ARG:HG2	1.98	0.63
1:A:279:ARG:N	1:A:279:ARG:HD2	2.14	0.63
1:A:353:GLN:HG3	4:A:786:HOH:O	1.98	0.63
1:A:37:THR:HG21	1:A:176:MET:HE1	1.80	0.62
1:A:308[B]:VAL:HG12	4:A:931:HOH:O	2.00	0.60
1:A:86:ARG:H	1:A:249:HIS:CD2	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:HG21	1:A:176:MET:CE	2.32	0.58
1:A:137:MET:CE	1:A:137:MET:CA	2.72	0.58
1:A:18:ASP:OD1	1:A:20:LYS:HG2	2.03	0.58
1:A:37:THR:HG22	1:A:39:GLY:N	2.06	0.58
1:A:78:GLY:C	1:A:137:MET:HE1	2.29	0.57
1:A:3:GLU:HG3	1:A:23:VAL:O	2.05	0.57
1:A:281:ALA:HB3	1:A:284:LEU:HB2	1.88	0.54
1:A:137:MET:HE2	1:A:137:MET:HA	1.87	0.54
1:A:60:ILE:HD12	1:A:64:LEU:HD23	1.90	0.54
1:A:137:MET:HE2	1:A:141:LEU:CD2	2.27	0.53
1:A:212:GLN:HE22	1:A:432:ARG:NE	2.06	0.53
1:A:289:TYR:O	1:A:293[B]:ARG:HG3	2.09	0.53
1:A:74[A]:ARG:HB2	1:A:74[A]:ARG:HH11	1.73	0.53
1:A:349:ARG:HH12	1:A:353:GLN:HG3	1.74	0.53
1:A:262:HIS:HD2	1:A:267:LEU:O	1.92	0.53
1:A:67:THR:HB	1:A:74[A]:ARG:HH11	1.74	0.52
1:A:276:ARG:HG2	4:A:1150:HOH:O	2.10	0.52
1:A:147:ARG:HD2	4:A:1005:HOH:O	2.08	0.52
1:A:420:GLU:HG3	4:A:1167:HOH:O	2.10	0.51
1:A:143:ALA:O	1:A:147:ARG:HG2	2.11	0.51
1:A:86:ARG:H	1:A:249:HIS:HD2	1.58	0.50
1:A:275:HIS:HD2	4:A:1169:HOH:O	1.94	0.49
1:A:137:MET:CE	1:A:141:LEU:CD2	2.89	0.49
1:A:262:HIS:CE1	1:A:391:GLU:OE2	2.61	0.49
1:A:524:ALA:O	1:A:528:GLU:HG3	2.12	0.49
1:A:118:HIS:HE1	1:A:202:LEU:HD21	1.76	0.49
1:A:485:GLN:HG3	1:A:486:GLU:HG2	1.95	0.48
1:A:522[A]:GLU:H	1:A:522[A]:GLU:CD	2.21	0.48
1:A:212:GLN:NE2	1:A:432:ARG:NE	2.62	0.48
1:A:262:HIS:CD2	1:A:267:LEU:O	2.68	0.47
1:A:350:PHE:CE2	1:A:357:ASN:HB3	2.50	0.47
1:A:118:HIS:CE1	1:A:202:LEU:HD21	2.49	0.46
1:A:136:GLU:O	1:A:137:MET:HE3	2.16	0.46
1:A:306:ASN:ND2	1:A:307:GLN:HG3	2.31	0.45
1:A:348:GLU:O	1:A:352:ARG:HG3	2.17	0.45
1:A:254:GLY:H	1:A:364:ASN:HD22	1.65	0.44
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.81	0.44
1:A:98:SER:HB3	1:A:118:HIS:HB2	1.99	0.43
1:A:65[A]:SER:OG	4:A:867:HOH:O	2.20	0.43
1:A:74[A]:ARG:HB2	1:A:74[A]:ARG:NH1	2.34	0.43
1:A:80:GLU:OE2	1:A:275:HIS:ND1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:HA	1:A:241:PRO:HD3	1.88	0.41
1:A:294:LEU:CD2	1:A:336:ALA:HA	2.50	0.41
1:A:603:GLN:HG2	4:A:1228:HOH:O	2.20	0.41
1:A:76:GLU:HA	1:A:85:VAL:O	2.21	0.41
1:A:284:LEU:HD22	1:A:289:TYR:CZ	2.56	0.41
1:A:349:ARG:NH1	1:A:353:GLN:HG3	2.34	0.41
1:A:80:GLU:HG3	4:A:1072:HOH:O	2.20	0.41
1:A:208:TYR:OH	1:A:241:PRO:HG3	2.21	0.41
1:A:175:VAL:HG21	1:A:223:LYS:HD2	2.03	0.40
1:A:462:LEU:HD12	1:A:463:ASP:O	2.21	0.40
1:A:498:LEU:HD23	1:A:498:LEU:HA	1.96	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	602/613 (98%)	586 (97%)	15 (2%)	1 (0%)	43 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	PRO

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	481/487 (99%)	476 (99%)	5 (1%)	68	42

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

Mol	Chain	Res	Type
1	A	80	GLU
1	A	137	MET
1	A	139	ASP
1	A	262	HIS
1	A	306	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	82	ASN
1	A	92	GLN
1	A	124	ASN
1	A	156	HIS
1	A	178	GLN
1	A	212	GLN
1	A	249	HIS
1	A	262	HIS
1	A	266	HIS
1	A	277	GLN
1	A	306	ASN
1	A	307	GLN
1	A	332	GLN
1	A	364	ASN
1	A	415[A]	GLN
1	A	483	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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	599/613 (97%)	0.65	82 (13%) 6 7	6, 18, 46, 89	9 (1%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547[A]	GLU	8.9
1	A	487	PRO	6.9
1	A	280	GLY	5.6
1	A	492	ARG	5.2
1	A	549	GLY	5.2
1	A	493	ILE	5.1
1	A	323	GLY	5.0
1	A	279	ARG	4.7
1	A	491	GLY	4.7
1	A	322	GLY	4.6
1	A	34	ILE	4.5
1	A	83	LYS	4.5
1	A	122	ALA	4.4
1	A	489	ALA	4.3
1	A	606	LYS	4.2
1	A	355	THR	4.1
1	A	356	GLY	4.1
1	A	354	GLY	4.0
1	A	462	LEU	4.0
1	A	415[A]	GLN	4.0
1	A	32	PRO	3.9
1	A	522[A]	GLU	3.5
1	A	129	MET	3.4
1	A	33	ALA	3.4
1	A	519	ALA	3.4
1	A	352	ARG	3.4
1	A	375	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	302	ARG	3.4
1	A	212	GLN	3.3
1	A	293[A]	ARG	3.2
1	A	301	ALA	3.2
1	A	239	ILE	3.1
1	A	488	ASP	3.1
1	A	107	HIS	3.1
1	A	240	LYS	3.0
1	A	281	ALA	3.0
1	A	124	ASN	3.0
1	A	74[A]	ARG	2.9
1	A	147	ARG	2.9
1	A	80	GLU	2.9
1	A	548	GLU	2.9
1	A	376	ALA	2.8
1	A	36	ASP	2.7
1	A	2	GLU	2.6
1	A	317	ALA	2.6
1	A	286	GLN	2.6
1	A	353	GLN	2.6
1	A	325	LEU	2.5
1	A	9	ASN	2.5
1	A	203	ASP	2.5
1	A	242	THR	2.5
1	A	427	ARG	2.5
1	A	276	ARG	2.5
1	A	146	ALA	2.4
1	A	148	ASP	2.4
1	A	200	ASP	2.4
1	A	463	ASP	2.4
1	A	241	PRO	2.3
1	A	383	ALA	2.3
1	A	8	TRP	2.3
1	A	294	LEU	2.3
1	A	516	LEU	2.3
1	A	326	GLY	2.3
1	A	185	LYS	2.3
1	A	161	MET	2.2
1	A	324	ASP	2.2
1	A	278	PRO	2.2
1	A	490	ARG	2.1
1	A	320	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	300	ALA	2.1
1	A	277	GLN	2.1
1	A	486	GLU	2.1
1	A	319	PRO	2.1
1	A	299	LEU	2.1
1	A	518	LEU	2.1
1	A	178	GLN	2.1
1	A	304	SER	2.1
1	A	39	GLY	2.1
1	A	521	PRO	2.1
1	A	37	THR	2.0
1	A	605	GLY	2.0
1	A	218	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 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
3	NA	A	704	1/1	0.90	0.20	30,30,30,30	0
2	CL	A	702	1/1	0.95	0.12	27,27,27,27	0
2	CL	A	701	1/1	0.98	0.07	17,17,17,17	0
3	NA	A	703	1/1	0.99	0.06	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.