



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2026 – 02:24 PM EDT

PDB ID : 9NX5 / pdb_00009nx5
Title : Crystal Structure of a P. Aeruginosa Gyrase
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Deposited on : 2025-03-25
Resolution : 2.40 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

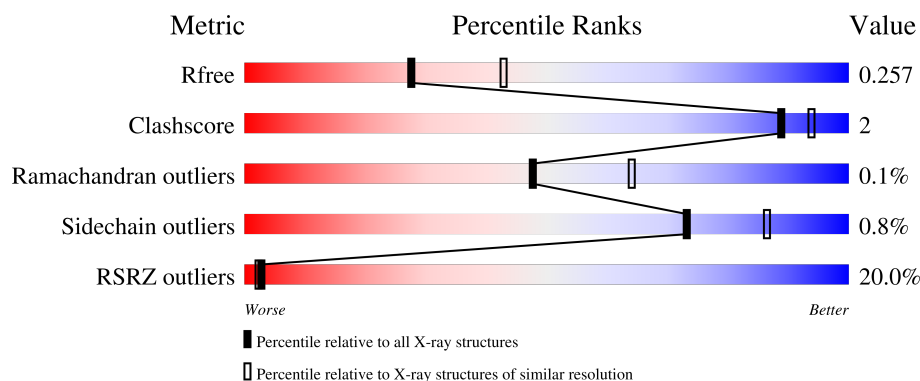
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	942	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13110 atoms, of which 6364 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 DNA gyrase subunit B,DNA gyrase subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	866	Total	C	H	N	O	S	0	9	0
			12900	4144	6322	1150	1256	28			

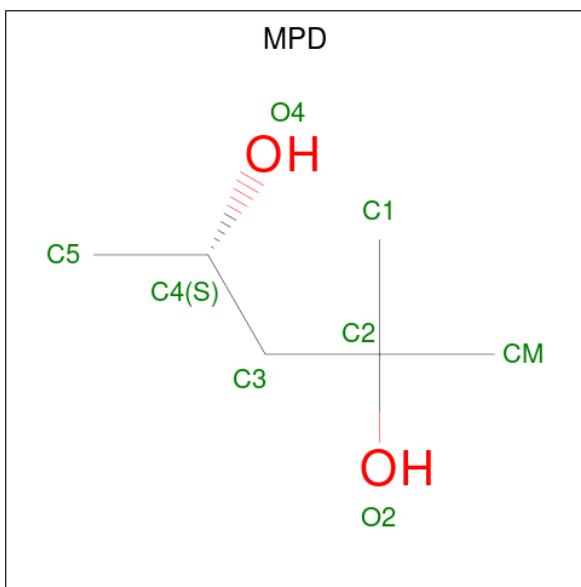
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	GLY	-	expression tag	UNP Q9S1C7
A	393	SER	-	expression tag	UNP Q9S1C7
A	394	ALA	-	expression tag	UNP Q9S1C7
A	395	ALA	-	expression tag	UNP Q9S1C7
A	396	ALA	-	expression tag	UNP Q9S1C7
A	999	GLY	-	linker	UNP Q9S1C7
A	1000	GLY	-	linker	UNP Q9S1C7
A	1001	SER	-	linker	UNP Q9S1C7

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			22	6	14	2		
3	A	1	Total	C	H	O	0	0
			22	6	14	2		
3	A	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

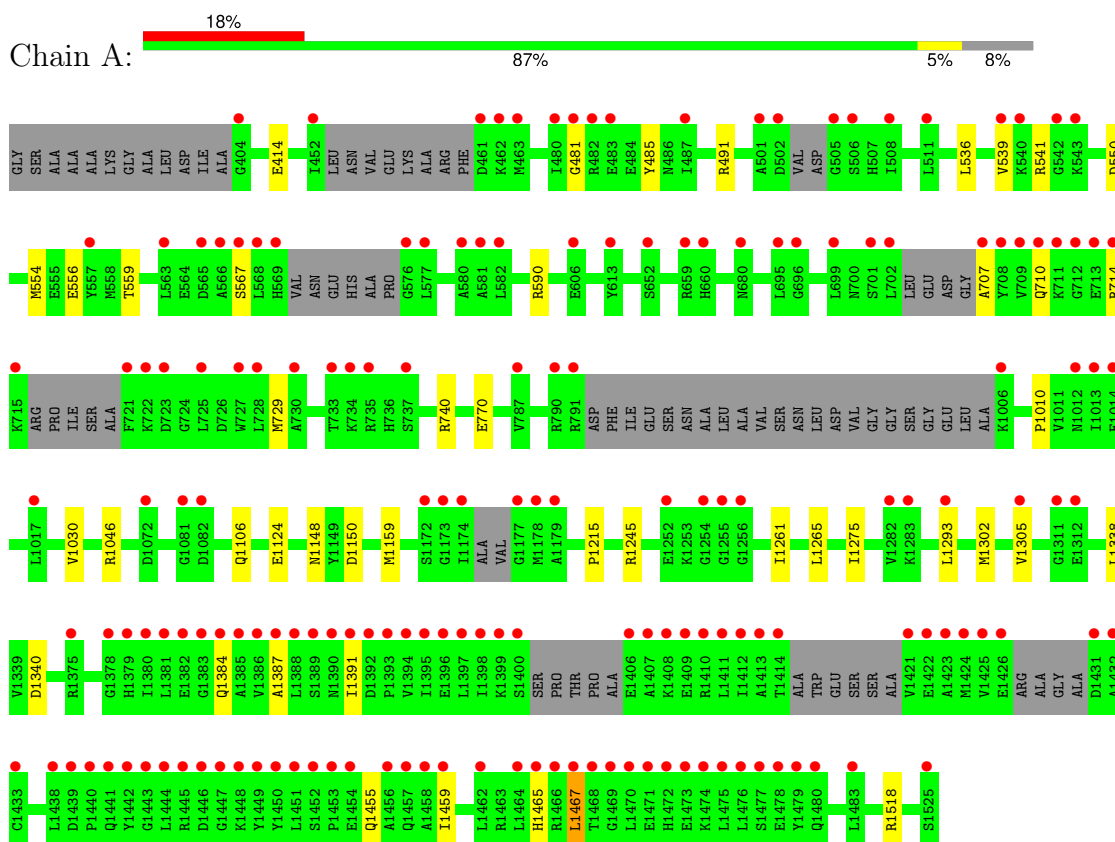
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total	O	0	0
			141	141		

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: DNA gyrase subunit B,DNA gyrase subunit A



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	218.16Å 218.16Å 108.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.76 – 2.40 48.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.76-2.40) 91.8 (48.76-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.242 , 0.257 0.242 , 0.257	Depositor DCC
R_{free} test set	2984 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13110	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: MPD, NA, CL

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	0.13	0/6713	0.29	0/9090

There are no bond length outliers.

There are no bond angle outliers.

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	6578	6322	6281	25	0
2	A	1	0	0	0	0
3	A	24	42	42	0	0
4	A	2	0	0	0	0
5	A	141	0	0	1	0
All	All	6746	6364	6323	25	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 2.

All (25) 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:1275:ILE:HG23	1:A:1293:LEU:HD13	1.81	0.62
1:A:1265:LEU:HG	1:A:1302:MET:HE1	1.82	0.62
1:A:556:GLU:OE1	1:A:590:ARG:NH2	2.33	0.61
1:A:1391:ILE:CD1	1:A:1467:LEU:HD21	2.31	0.60
1:A:539:VAL:HG11	1:A:554:MET:HE1	1.82	0.60
1:A:1261:ILE:HD12	1:A:1305:VAL:HG22	1.84	0.59
1:A:481:GLY:O	1:A:485:TYR:N	2.32	0.58
1:A:707:ALA:O	1:A:714:ARG:N	2.36	0.57
1:A:1030:VAL:HG12	1:A:1338:LEU:HD21	1.86	0.57
1:A:740:ARG:NH2	1:A:1010:PRO:O	2.38	0.56
1:A:1293:LEU:HD12	1:A:1293:LEU:O	2.06	0.55
1:A:1215:PRO:O	1:A:1518:ARG:NH2	2.43	0.51
1:A:1455:GLN:O	1:A:1459:ILE:N	2.41	0.49
1:A:559:THR:OG1	1:A:729:MET:HE1	2.12	0.48
1:A:770:GLU:OE1	1:A:770:GLU:N	2.45	0.48
1:A:1391:ILE:HD11	1:A:1467:LEU:HD21	1.95	0.47
1:A:414:GLU:O	1:A:491:ARG:NH2	2.45	0.47
1:A:1046:ARG:HG2	1:A:1159:MET:HE2	1.98	0.46
1:A:1261:ILE:CD1	1:A:1305:VAL:HG22	2.44	0.46
1:A:536:LEU:HD12	1:A:550:ASP:HA	1.99	0.45
1:A:1245:ARG:NH2	5:A:1706:HOH:O	2.42	0.44
1:A:1384:GLN:O	1:A:1387:ALA:HB3	2.18	0.44
1:A:1293:LEU:HD12	1:A:1293:LEU:C	2.43	0.44
1:A:1106:GLN:NE2	1:A:1124:GLU:OE1	2.51	0.42
1:A:1148:ASN:ND2	1:A:1150:ASP:OD1	2.53	0.41

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	853/942 (91%)	844 (99%)	8 (1%)	1 (0%)	48 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	710	GLN

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	654/786 (83%)	649 (99%)	5 (1%)	73 86

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

Mol	Chain	Res	Type
1	A	541	ARG
1	A	567	SER
1	A	1340	ASP
1	A	1465	HIS
1	A	1467	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1019	GLN
1	A	1319	ASN
1	A	1328	GLN
1	A	1379	HIS
1	A	1390	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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z > 2$
3	MPD	A	1602	-	7,7,7	0.33	0	9,10,10	0.29	0
3	MPD	A	1604	-	7,7,7	0.34	0	9,10,10	0.28	0
3	MPD	A	1603	-	7,7,7	0.33	0	9,10,10	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
3	MPD	A	1602	-	-	1/5/5/5	-
3	MPD	A	1604	-	-	0/5/5/5	-
3	MPD	A	1603	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1602	MPD	O2-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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	866/942 (91%)	1.12	173 (19%) 3 2	31, 69, 162, 208	4 (0%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1426	GLU	10.8
1	A	715	LYS	8.3
1	A	1421	VAL	8.2
1	A	1422	GLU	8.0
1	A	1449	TYR	7.0
1	A	569	HIS	7.0
1	A	1470	LEU	6.8
1	A	1400	SER	6.7
1	A	1394	VAL	6.7
1	A	1446	ASP	6.5
1	A	452	ILE	6.5
1	A	1444	LEU	6.5
1	A	1177	GLY	6.3
1	A	1414	THR	6.3
1	A	1006	LYS	6.3
1	A	502	ASP	6.2
1	A	505	GLY	5.9
1	A	1387	ALA	5.9
1	A	461	ASP	5.9
1	A	1471	GLU	5.8
1	A	1441	GLN	5.7
1	A	1423	ALA	5.5
1	A	1445	ARG	5.5
1	A	707	ALA	5.4
1	A	1408	LYS	5.3
1	A	1388	LEU	5.2
1	A	713	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	483	GLU	5.1
1	A	1464	LEU	5.0
1	A	1173	GLY	5.0
1	A	1432	ALA	4.9
1	A	723	ASP	4.9
1	A	1450	TYR	4.9
1	A	1473	GLU	4.9
1	A	1433	CYS	4.9
1	A	1448	LYS	4.9
1	A	1472	HIS	4.8
1	A	1475	LEU	4.8
1	A	1410	ARG	4.7
1	A	1425	VAL	4.6
1	A	1255	GLY	4.6
1	A	1407	ALA	4.6
1	A	1398	ILE	4.6
1	A	1474	LYS	4.6
1	A	1391	ILE	4.5
1	A	721	PHE	4.5
1	A	1389	SER	4.5
1	A	1178	MET	4.5
1	A	701	SER	4.4
1	A	576	GLY	4.4
1	A	1393	PRO	4.4
1	A	1477	SER	4.4
1	A	506	SER	4.4
1	A	1525	SER	4.3
1	A	1447	GLY	4.3
1	A	1467	LEU	4.3
1	A	1392	ASP	4.3
1	A	482	ARG	4.3
1	A	511	LEU	4.3
1	A	462	LYS	4.2
1	A	695	LEU	4.2
1	A	1386	VAL	4.2
1	A	1411	LEU	4.2
1	A	1397	LEU	4.2
1	A	1469	GLY	4.1
1	A	1466	ARG	4.1
1	A	1082	ASP	4.1
1	A	1409	GLU	4.1
1	A	1406	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	404	GLY	4.0
1	A	1399	LYS	4.0
1	A	1476	LEU	4.0
1	A	702	LEU	4.0
1	A	1312[A]	GLU	4.0
1	A	1459	ILE	3.9
1	A	1172	SER	3.9
1	A	1174	ILE	3.9
1	A	1385	ALA	3.8
1	A	1458	ALA	3.8
1	A	1468	THR	3.8
1	A	577	LEU	3.8
1	A	1424	MET	3.8
1	A	699	LEU	3.7
1	A	1451	LEU	3.7
1	A	1462	LEU	3.7
1	A	1431	ASP	3.7
1	A	1457	GLN	3.7
1	A	1254	GLY	3.6
1	A	1378	GLY	3.6
1	A	1412	ILE	3.6
1	A	1252	GLU	3.6
1	A	1396	GLU	3.5
1	A	1479	TYR	3.5
1	A	714	ARG	3.5
1	A	708	TYR	3.5
1	A	791	ARG	3.5
1	A	487	ILE	3.5
1	A	543	LYS	3.5
1	A	463	MET	3.4
1	A	1390	ASN	3.4
1	A	565	ASP	3.3
1	A	1380	ILE	3.3
1	A	1256	GLY	3.3
1	A	1305	VAL	3.3
1	A	501	ALA	3.2
1	A	539	VAL	3.2
1	A	481	GLY	3.2
1	A	712	GLY	3.2
1	A	1395	ILE	3.2
1	A	722	LYS	3.2
1	A	1440	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	659	ARG	3.1
1	A	1382	GLU	3.1
1	A	1454	GLU	3.1
1	A	1452	SER	3.1
1	A	735	ARG	3.1
1	A	790	ARG	3.0
1	A	696	GLY	3.0
1	A	1014	GLU	2.9
1	A	1282	VAL	2.9
1	A	711	LYS	2.9
1	A	727	TRP	2.9
1	A	1439	ASP	2.9
1	A	1383	GLY	2.9
1	A	710	GLN	2.9
1	A	1465	HIS	2.8
1	A	542	GLY	2.8
1	A	1072	ASP	2.8
1	A	568	LEU	2.8
1	A	1480	GLN	2.8
1	A	1384	GLN	2.8
1	A	540	LYS	2.7
1	A	557	TYR	2.7
1	A	1456	ALA	2.7
1	A	563	LEU	2.7
1	A	725	LEU	2.6
1	A	1081	GLY	2.6
1	A	1453	PRO	2.6
1	A	1293	LEU	2.6
1	A	613	TYR	2.6
1	A	709	VAL	2.5
1	A	787	VAL	2.5
1	A	1442	TYR	2.5
1	A	1311	GLY	2.5
1	A	1443	GLY	2.5
1	A	582	LEU	2.5
1	A	1179	ALA	2.5
1	A	1438	LEU	2.4
1	A	1483	LEU	2.4
1	A	652	SER	2.4
1	A	580	ALA	2.4
1	A	567	SER	2.3
1	A	1379	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1381	LEU	2.3
1	A	680	ASN	2.3
1	A	480	ILE	2.3
1	A	508	ILE	2.3
1	A	1017	LEU	2.3
1	A	1012	ASN	2.2
1	A	1013	ILE	2.2
1	A	1375	ARG	2.2
1	A	566	ALA	2.2
1	A	734	LYS	2.2
1	A	660	HIS	2.2
1	A	733	THR	2.2
1	A	1413	ALA	2.1
1	A	1283	LYS	2.1
1	A	728	LEU	2.1
1	A	581	ALA	2.1
1	A	606	GLU	2.0
1	A	1478	GLU	2.0
1	A	730	ALA	2.0
1	A	737	SER	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(\AA^2)	Q<0.9
3	MPD	A	1604	8/8	0.80	0.20	46,64,75,80	0
3	MPD	A	1603	8/8	0.83	0.18	51,66,77,79	0
4	CL	A	1605	1/1	0.88	0.13	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MPD	A	1602	8/8	0.89	0.21	48,58,61,66	0
4	CL	A	1606	1/1	0.90	0.12	88,88,88,88	0
2	NA	A	1601	1/1	0.93	0.07	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.