



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:04 PM UTC

PDB ID : 1ZEF / pdb_00001zef
Title : structure of alkaline phosphatase from human placenta in complex with its uncompetitive inhibitor L-Phe
Authors : Llinas, P.; Stura, E.A.; Menez, A.; Kiss, Z.; Stigbrand, T.; Millan, J.L.; Le Du, M.H.
Deposited on : 2005-04-18
Resolution : 1.90 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

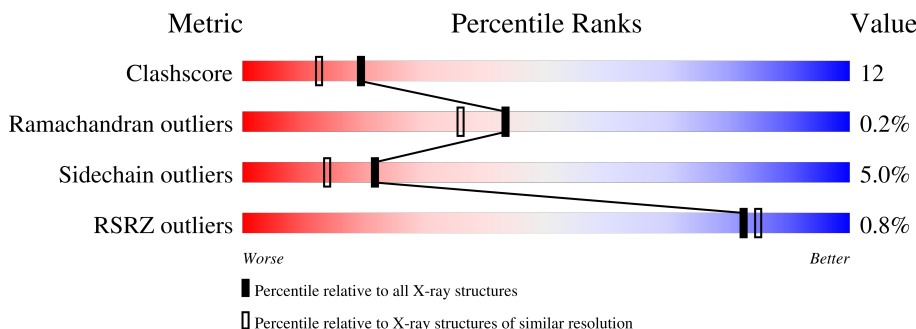
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	484	82% 15% ...

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
3	PHE	A	802	-	-	X	-
3	PHE	A	804	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4427 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 Alkaline phosphatase.

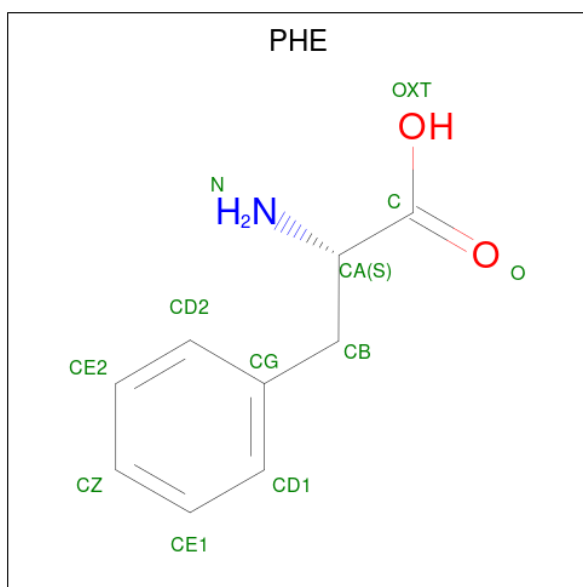
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	P	S	0	0	0
			3669	2292	653	705	1	18			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	A	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

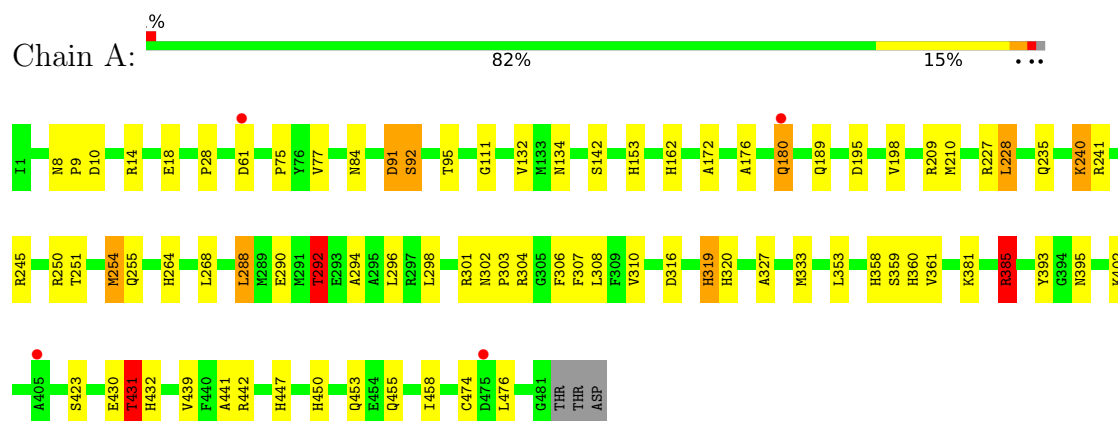
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	702	Total 702	O 702	0	0

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: Alkaline phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.79Å 114.94Å 106.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90 15.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-1.90) 98.4 (15.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.126 , 0.173 0.141 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 60.9	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	0.97	EDS
Total number of atoms	4427	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: MG, SEP, NAG, CA, ZN

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	0.99	1/3739 (0.0%)	1.00	8/5072 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	MET	SD-CE	-5.22	1.66	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	CYS	CA-C-N	-9.72	106.82	122.95
1	A	474	CYS	C-N-CA	-9.72	106.82	122.95
1	A	474	CYS	N-CA-C	-8.14	99.76	110.43
1	A	431	THR	N-CA-CB	-6.81	99.52	110.63
1	A	385	ARG	CG-CD-NE	5.83	124.82	112.00
1	A	319	HIS	N-CA-CB	5.36	118.00	110.12
1	A	431	THR	CA-CB-CG2	5.19	119.32	110.50
1	A	292	THR	CA-CB-OG1	5.14	117.31	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	ASP	Peptide

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	3669	0	3549	77	0
2	A	28	0	26	1	0
3	A	24	0	16	13	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	702	0	0	23	5
All	All	4427	0	3591	85	5

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 12.

All (85) 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:333:MET:HE2	7:A:1591:HOH:O	1.39	1.22
1:A:453:GLN:HG3	7:A:1054:HOH:O	1.51	1.09
1:A:92:SEP:P	3:A:802:PHE:N	2.35	0.99
3:A:804:PHE:HD1	3:A:804:PHE:O	1.51	0.94
3:A:804:PHE:O	3:A:804:PHE:CD1	2.20	0.94
1:A:301:ARG:NH2	7:A:1592:HOH:O	1.91	0.88
1:A:176:ALA:O	1:A:180:GLN:HG2	1.76	0.86
1:A:162:HIS:H	1:A:189:GLN:HE22	1.25	0.85
3:A:802:PHE:HE1	7:A:1595:HOH:O	1.64	0.79
1:A:333:MET:HB2	7:A:1591:HOH:O	1.84	0.77
1:A:431:THR:HG23	1:A:432:HIS:O	1.86	0.75
1:A:288:LEU:O	1:A:292:THR:HG23	1.90	0.71
1:A:360:HIS:HD2	1:A:430:GLU:OE1	1.75	0.70
2:A:801:NAG:O6	7:A:1513:HOH:O	2.10	0.69
1:A:450:HIS:HE1	7:A:985:HOH:O	1.76	0.68
1:A:333:MET:SD	7:A:1508:HOH:O	2.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:HIS:CE1	1:A:327:ALA:CB	2.79	0.65
1:A:264:HIS:CE1	7:A:1247:HOH:O	2.48	0.65
3:A:804:PHE:CD1	3:A:804:PHE:C	2.75	0.64
1:A:172:ALA:HA	1:A:228:LEU:HD22	1.79	0.64
1:A:153:HIS:HD2	7:A:957:HOH:O	1.83	0.60
1:A:28:PRO:CB	1:A:447:HIS:CE1	2.85	0.59
1:A:360:HIS:CD2	1:A:430:GLU:OE1	2.55	0.58
1:A:302:ASN:ND2	1:A:304:ARG:H	2.01	0.58
1:A:28:PRO:HB3	1:A:447:HIS:ND1	2.19	0.57
1:A:302:ASN:HD22	1:A:302:ASN:C	2.12	0.57
1:A:8:ASN:C	1:A:8:ASN:HD22	2.12	0.56
1:A:111:GLY:O	1:A:162:HIS:HD2	1.88	0.56
1:A:195:ASP:OD1	1:A:264:HIS:HE1	1.89	0.56
1:A:319:HIS:CE1	1:A:327:ALA:HB1	2.41	0.56
1:A:381:LYS:NZ	7:A:1265:HOH:O	2.38	0.55
1:A:209:ARG:HG2	7:A:1221:HOH:O	2.07	0.54
3:A:802:PHE:N	3:A:802:PHE:CD2	2.74	0.54
1:A:393:TYR:O	1:A:423:SER:HA	2.07	0.54
1:A:8:ASN:ND2	1:A:10:ASP:H	2.07	0.53
1:A:358:HIS:HD2	1:A:359:SER:O	1.91	0.53
1:A:385:ARG:HG2	1:A:385:ARG:HH21	1.73	0.53
1:A:8:ASN:HD22	1:A:9:PRO:N	2.07	0.52
1:A:28:PRO:HB3	1:A:447:HIS:CE1	2.44	0.52
1:A:385:ARG:NE	7:A:1469:HOH:O	2.43	0.52
1:A:320:HIS:CD2	3:A:802:PHE:HA	2.32	0.52
1:A:254:MET:HA	3:A:804:PHE:CZ	2.45	0.51
3:A:804:PHE:N	7:A:1575:HOH:O	2.43	0.51
1:A:302:ASN:HD22	1:A:303:PRO:N	2.08	0.51
1:A:162:HIS:HE1	7:A:1063:HOH:O	1.94	0.50
3:A:802:PHE:N	3:A:802:PHE:HD2	2.08	0.50
1:A:28:PRO:HB2	1:A:447:HIS:CE1	2.45	0.50
1:A:84:ASN:HD21	1:A:91:ASP:H	1.59	0.49
1:A:255:GLN:NE2	7:A:1172:HOH:O	2.44	0.49
1:A:353:LEU:HD12	1:A:458:ILE:HG23	1.94	0.49
1:A:439:VAL:HG21	1:A:458:ILE:HD11	1.95	0.49
1:A:92:SEP:O1P	3:A:802:PHE:N	2.40	0.47
1:A:447:HIS:CD2	1:A:447:HIS:C	2.92	0.47
1:A:251:THR:HG23	7:A:1053:HOH:O	2.15	0.47
1:A:28:PRO:CB	1:A:447:HIS:ND1	2.78	0.46
1:A:302:ASN:HD22	1:A:304:ARG:H	1.63	0.45
1:A:18:GLU:OE2	7:A:1487:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HA	1:A:439:VAL:O	2.16	0.45
1:A:307:PHE:C	1:A:307:PHE:CD1	2.95	0.45
1:A:209:ARG:HA	1:A:227:ARG:HB2	1.99	0.45
1:A:14:ARG:HD2	7:A:1366:HOH:O	2.16	0.45
1:A:162:HIS:H	1:A:189:GLN:NE2	2.04	0.45
1:A:195:ASP:OD1	1:A:264:HIS:CE1	2.69	0.45
1:A:316:ASP:OD2	1:A:360:HIS:CE1	2.70	0.45
1:A:95:THR:HG22	1:A:455:GLN:HE22	1.83	0.44
1:A:316:ASP:OD2	1:A:360:HIS:HE1	2.01	0.44
1:A:319:HIS:ND1	1:A:327:ALA:CB	2.82	0.43
1:A:290:GLU:HG2	3:A:804:PHE:C	2.45	0.42
1:A:320:HIS:HE1	1:A:432:HIS:CD2	2.38	0.42
1:A:353:LEU:HD22	1:A:441:ALA:HB2	2.02	0.42
1:A:198:VAL:HG22	1:A:298:LEU:HD13	2.02	0.42
1:A:294:ALA:HB2	3:A:804:PHE:CZ	2.53	0.42
1:A:75:PRO:HD2	1:A:442:ARG:HB3	2.02	0.41
1:A:308:LEU:HG	1:A:310:VAL:HG23	2.02	0.41
1:A:153:HIS:CD2	7:A:957:HOH:O	2.66	0.41
1:A:142:SER:O	1:A:306:PHE:HA	2.21	0.41
1:A:288:LEU:O	1:A:292:THR:CG2	2.65	0.41
1:A:320:HIS:CE1	1:A:432:HIS:CD2	3.08	0.41
1:A:251:THR:HB	7:A:1461:HOH:O	2.21	0.41
1:A:333:MET:CE	7:A:1508:HOH:O	2.68	0.41
1:A:395:ASN:HD21	1:A:431:THR:CG2	2.33	0.41
1:A:240:LYS:HD3	7:A:1153:HOH:O	2.21	0.41
1:A:250:ARG:O	1:A:254:MET:HG3	2.21	0.40
1:A:8:ASN:HD22	1:A:9:PRO:CD	2.34	0.40
1:A:319:HIS:HD2	1:A:360:HIS:HB2	1.87	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1068:HOH:O	7:A:1068:HOH:O[3_655]	1.34	0.86
7:A:1042:HOH:O	7:A:1570:HOH:O[3_655]	1.93	0.27
7:A:1062:HOH:O	7:A:1062:HOH:O[3_655]	1.94	0.26
7:A:1439:HOH:O	7:A:1548:HOH:O[3_655]	1.95	0.25
7:A:1089:HOH:O	7:A:1429:HOH:O[3_655]	2.17	0.03

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	478/484 (99%)	468 (98%)	9 (2%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	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	A	377/386 (98%)	359 (95%)	18 (5%)	23	15

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASP
1	A	132	VAL
1	A	134	ASN
1	A	180	GLN
1	A	228	LEU
1	A	235	GLN
1	A	240	LYS
1	A	241	ARG
1	A	245	ARG
1	A	254	MET

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Mol	Chain	Res	Type
1	A	268	LEU
1	A	288	LEU
1	A	292	THR
1	A	296	LEU
1	A	385	ARG
1	A	402	LYS
1	A	431	THR
1	A	476	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	84	ASN
1	A	127	ASN
1	A	134	ASN
1	A	153	HIS
1	A	162	HIS
1	A	180	GLN
1	A	189	GLN
1	A	193	ASN
1	A	255	GLN
1	A	264	HIS
1	A	302	ASN
1	A	358	HIS
1	A	360	HIS
1	A	450	HIS
1	A	455	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
1	SEP	A	92	4,1	8,9,10	1.77	1 (12%)	7,12,14	2.28	2 (28%)

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
1	SEP	A	92	4,1	-	1/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	SEP	P-OG	4.59	1.74	1.60

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	SEP	O3P-P-OG	-4.93	93.81	106.67
1	A	92	SEP	O3P-P-O2P	2.29	116.38	107.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	92	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	92	SEP	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	NAG	A	801	1	14,14,15	0.73	0	17,19,21	1.25	2 (11%)
3	PHE	A	804	-	11,12,12	1.44	2 (18%)	11,15,15	2.44	1 (9%)
2	NAG	A	803	1	14,14,15	0.67	0	17,19,21	2.26	4 (23%)
3	PHE	A	802	4	11,12,12	0.97	0	11,15,15	1.76	2 (18%)

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	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	PHE	A	804	-	-	4/8/8/8	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	PHE	A	802	4	-	6/8/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	PHE	CE2-CD2	-3.01	1.33	1.38
3	A	804	PHE	CE1-CD1	-2.69	1.34	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	804	PHE	OXT-C-O	-7.92	106.12	124.08
2	A	803	NAG	C1-O5-C5	5.69	119.82	112.19
2	A	803	NAG	O5-C1-C2	-5.18	103.28	111.29
3	A	802	PHE	OXT-C-O	-4.57	113.71	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	803	NAG	C6-C5-C4	-3.04	105.56	113.02
2	A	801	NAG	O5-C1-C2	-2.41	107.56	111.29
2	A	803	NAG	O6-C6-C5	-2.22	103.78	111.33
2	A	801	NAG	O7-C7-C8	-2.11	118.30	122.05
3	A	802	PHE	CB-CG-CD2	2.11	124.82	120.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	PHE	O-C-CA-N
3	A	802	PHE	N-CA-CB-CG
3	A	802	PHE	C-CA-CB-CG
3	A	804	PHE	C-CA-CB-CG
3	A	802	PHE	CA-CB-CG-CD2
3	A	802	PHE	CA-CB-CG-CD1
3	A	804	PHE	CA-CB-CG-CD1
3	A	804	PHE	CA-CB-CG-CD2
3	A	802	PHE	OXT-C-CA-N
3	A	804	PHE	OXT-C-CA-CB

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	1	0
3	A	804	PHE	7	0
3	A	802	PHE	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	480/484 (99%)	-0.50	4 (0%) 82 85	12, 18, 33, 49	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	ASP	4.3
1	A	475	ASP	3.0
1	A	180	GLN	2.5
1	A	405	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	92	10/11	0.99	0.04	13,14,15,15	0

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	PHE	A	804	12/12	0.67	0.17	47,48,49,50	0
2	NAG	A	803	14/15	0.77	0.11	31,37,40,46	0
3	PHE	A	802	12/12	0.79	0.20	39,44,49,49	0
2	NAG	A	801	14/15	0.82	0.11	27,39,47,48	0
4	ZN	A	901	1/1	1.00	0.03	14,14,14,14	0
4	ZN	A	902	1/1	1.00	0.01	15,15,15,15	0
5	MG	A	903	1/1	1.00	0.04	13,13,13,13	0
6	CA	A	904	1/1	1.00	0.01	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.