



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:53 AM UTC

PDB ID : 2ENX / pdb_00002enx
Title : Structure of the family II inorganic pyrophosphatase from *Streptococcus agalactiae* at 2.8 resolution
Authors : Rantanen, M.K.; Lehtio, L.; Rajagopal, L.; Rubens, C.E.; Goldman, A.
Deposited on : 2007-03-28
Resolution : 2.80 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

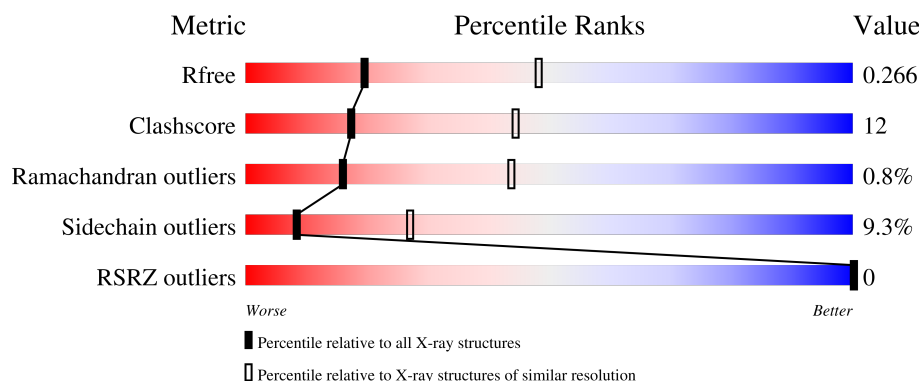
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	A	310	71% 25% .
1	B	310	75% 20% 5%

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
5	TRP	B	2031	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4923 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 Manganese-dependent inorganic pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2357	1489	384	479	5			
1	B	310	Total	C	N	O	S	0	0	0
			2357	1489	384	479	5			

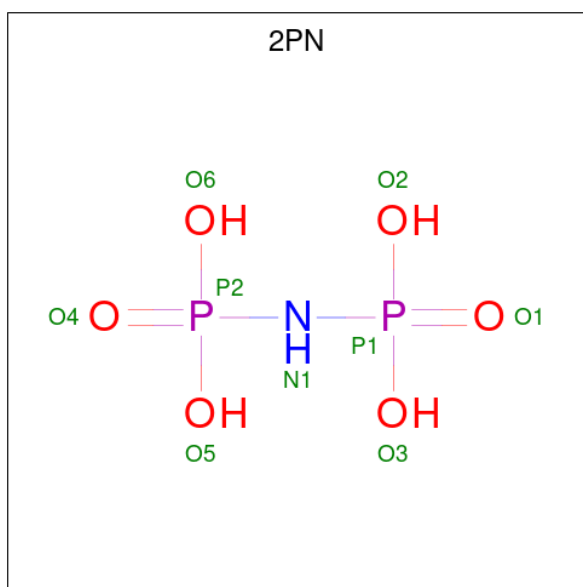
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

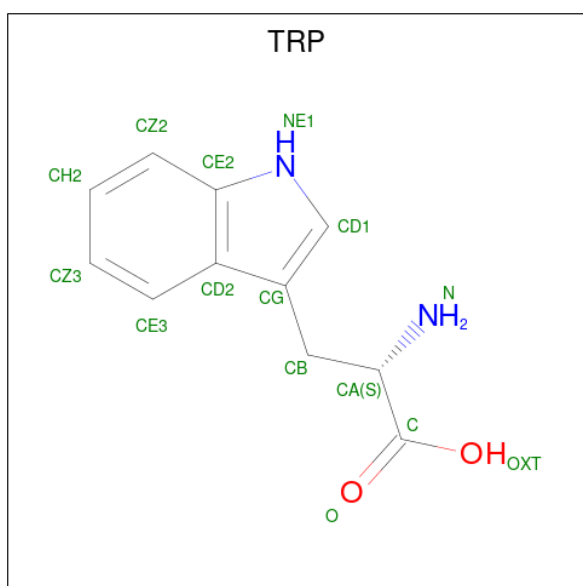
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is IMIDODIPHOSPHORIC ACID (CCD ID: 2PN) (formula: H₅NO₆P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	N	O	P	0	0
			9	1	6	2		
4	B	1	Total	N	O	P	0	0
			9	1	6	2		

- Molecule 5 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	11	2	2		
5	B	1	Total	C	N	O	0	0
			15	11	2	2		

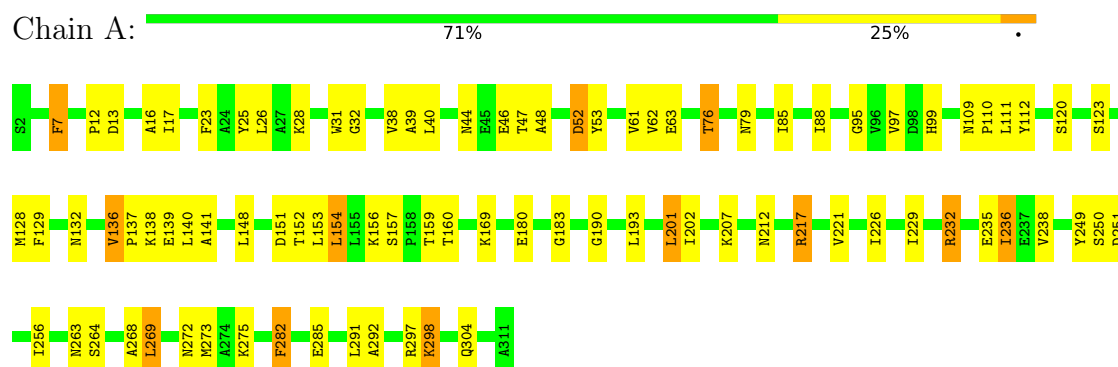
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	69	Total 69	O 69	0	0
6	B	86	Total 86	O 86	0	0

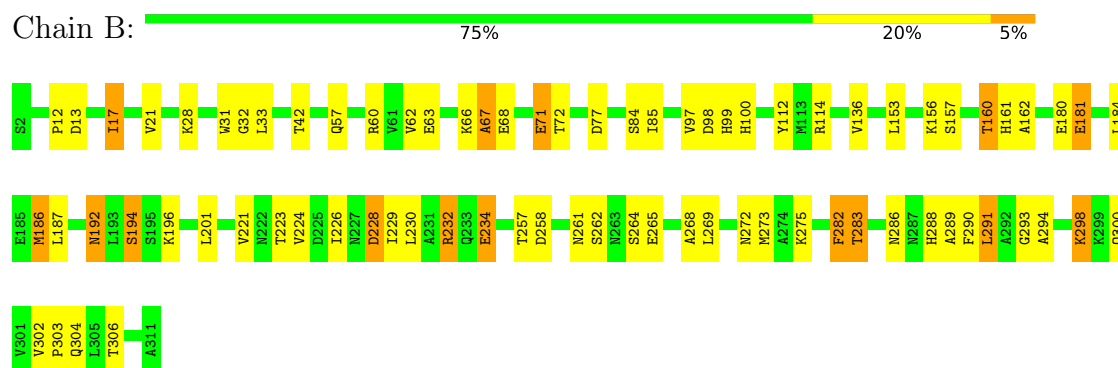
3 Residue-property plots

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: Manganese-dependent inorganic pyrophosphatase



- Molecule 1: Manganese-dependent inorganic pyrophosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	181.96Å 181.96Å 132.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.50 – 2.80 19.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.50-2.80) 99.1 (19.50-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.58 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.267 0.192 , 0.266	Depositor DCC
R_{free} test set	1036 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 19.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4923	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: 2PN, MN, MG

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	0.76	0/2393	1.03	5/3254 (0.2%)
1	B	0.78	0/2393	1.02	2/3254 (0.1%)
All	All	0.77	0/4786	1.03	7/6508 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	PHE	N-CA-C	6.90	119.56	109.07
1	A	151	ASP	N-CA-C	6.57	119.26	111.71
1	B	223	THR	N-CA-C	5.93	117.98	109.14
1	A	136	VAL	CA-C-N	-5.66	114.12	119.89
1	A	136	VAL	C-N-CA	-5.66	114.12	119.89
1	B	13	ASP	N-CA-C	-5.42	102.14	109.95
1	A	256	ILE	N-CA-C	5.30	111.88	106.21

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	2357	0	2332	59	0
1	B	2357	0	2332	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	9	0	1	3	0
4	B	9	0	1	1	0
5	A	15	0	9	4	0
5	B	15	0	9	6	0
6	A	69	0	0	6	0
6	B	86	0	0	12	0
All	All	4923	0	4684	118	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 12.

All (118) 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:B:232:ARG:HH21	1:B:232:ARG:HG2	1.33	0.94
1:B:66:LYS:HB2	6:B:2059:HOH:O	1.69	0.93
1:B:112:TYR:OH	5:B:2031:TRP:HA	1.73	0.88
1:A:232:ARG:HG2	1:A:232:ARG:HH21	1.36	0.88
1:B:262:SER:O	1:B:293:GLY:HA2	1.75	0.86
1:B:57:GLN:HB3	6:B:2082:HOH:O	1.81	0.79
1:B:234:GLU:HB2	6:B:2076:HOH:O	1.82	0.78
1:A:63:GLU:HA	1:A:63:GLU:OE1	1.85	0.75
1:B:71:GLU:HG3	6:B:2116:HOH:O	1.88	0.74
1:B:258:ASP:OD1	1:B:261:ASN:HB2	1.88	0.73
1:A:298:LYS:HE2	4:A:1001:2PN:HN1	1.56	0.70
1:A:112:TYR:CZ	5:A:1031:TRP:HB3	2.29	0.68
1:B:112:TYR:CZ	5:B:2031:TRP:HA	2.28	0.67
1:A:232:ARG:HH21	1:A:232:ARG:CG	2.07	0.67
1:A:31:TRP:CE3	5:A:1031:TRP:HA	2.31	0.66
1:A:298:LYS:HB3	4:A:1001:2PN:O1	1.98	0.63
1:B:112:TYR:HH	5:B:2031:TRP:HA	1.61	0.63
1:B:180:GLU:HG2	6:B:2115:HOH:O	2.00	0.62
1:B:31:TRP:HB2	1:B:33:LEU:HG	1.82	0.61
1:A:13:ASP:H	1:A:16:ALA:HB3	1.64	0.61
1:A:31:TRP:CD2	5:A:1031:TRP:HA	2.35	0.61
1:A:232:ARG:HG2	1:A:232:ARG:NH2	2.14	0.61
1:A:193:LEU:HD12	1:A:229:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HG2	1:A:249:TYR:CE2	2.37	0.59
1:B:98:ASP:OD2	1:B:99:HIS:N	2.34	0.59
1:A:99:HIS:CE1	1:A:120:SER:HA	2.36	0.59
1:B:282:PHE:HD1	1:B:282:PHE:C	2.11	0.59
1:B:232:ARG:HH21	1:B:232:ARG:CG	2.12	0.59
1:B:232:ARG:HG2	1:B:232:ARG:NH2	2.10	0.57
1:B:294:ALA:HA	1:B:300:GLN:NE2	2.20	0.57
1:B:282:PHE:C	1:B:282:PHE:CD1	2.84	0.56
1:B:229:ILE:N	1:B:229:ILE:HD12	2.19	0.56
1:A:7:PHE:HB3	1:A:38:VAL:O	2.06	0.56
5:B:2031:TRP:HD1	5:B:2031:TRP:O	1.90	0.55
1:B:272:ASN:HB3	1:B:275:LYS:HG3	1.88	0.55
1:B:262:SER:O	1:B:293:GLY:CA	2.54	0.55
1:B:28:LYS:O	1:B:32:GLY:HA2	2.08	0.54
1:B:181:GLU:HG3	6:B:2091:HOH:O	2.08	0.53
1:A:156:LYS:HE3	6:A:1092:HOH:O	2.09	0.53
1:A:12:PRO:HB2	1:A:17:ILE:HD11	1.91	0.53
1:B:273:MET:HA	1:B:273:MET:HE2	1.91	0.53
1:A:297:ARG:N	6:A:1085:HOH:O	2.28	0.52
1:B:62:VAL:HG11	1:B:68:GLU:HG3	1.92	0.52
1:A:201:LEU:HD13	1:A:221:VAL:HG11	1.92	0.52
1:B:62:VAL:HG12	1:B:63:GLU:N	2.24	0.52
1:A:23:PHE:HE1	1:A:128:MET:HE1	1.75	0.51
1:B:157:SER:O	1:B:160:THR:HB	2.10	0.51
1:B:226:ILE:HG22	1:B:230:LEU:HD12	1.91	0.51
1:B:273:MET:HG3	6:B:2077:HOH:O	2.10	0.51
1:A:180:GLU:OE2	1:A:180:GLU:HA	2.10	0.50
5:B:2031:TRP:O	5:B:2031:TRP:CD1	2.65	0.50
1:A:25:TYR:HB2	6:A:1056:HOH:O	2.11	0.49
1:A:39:ALA:O	1:A:61:VAL:HA	2.12	0.49
1:A:112:TYR:CE2	5:A:1031:TRP:HB3	2.47	0.49
1:A:298:LYS:HE2	4:A:1001:2PN:N1	2.25	0.49
1:B:77:ASP:OD2	1:B:100:HIS:HE1	1.95	0.49
1:A:76:THR:HA	1:A:97:VAL:O	2.13	0.48
1:B:153:LEU:O	1:B:156:LYS:HG3	2.14	0.48
1:A:232:ARG:O	1:A:236:ILE:HG13	2.13	0.48
1:A:95:GLY:HA2	1:A:112:TYR:O	2.14	0.48
1:A:40:LEU:HD21	1:A:85:ILE:HG13	1.95	0.47
1:B:265:GLU:OE1	1:B:288:HIS:ND1	2.47	0.47
1:A:26:LEU:HD13	1:A:129:PHE:HA	1.95	0.47
1:A:148:LEU:O	1:A:152:THR:OG1	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLN:OE1	1:A:304:GLN:N	2.47	0.47
1:A:273:MET:HE2	1:A:273:MET:HA	1.96	0.47
1:A:111:LEU:H	1:A:111:LEU:HD23	1.80	0.46
1:A:23:PHE:HE1	1:A:128:MET:CE	2.28	0.46
1:A:190:GLY:HA3	6:A:1078:HOH:O	2.14	0.46
1:A:263:ASN:OD1	1:A:292:ALA:HA	2.15	0.46
1:B:97:VAL:HG22	1:B:114:ARG:HB3	1.98	0.46
1:A:272:ASN:HB3	1:A:275:LYS:HG3	1.97	0.46
1:B:97:VAL:HA	1:B:114:ARG:O	2.16	0.46
1:A:153:LEU:O	1:A:156:LYS:HG2	2.15	0.46
1:B:66:LYS:O	1:B:67:ALA:C	2.59	0.46
1:B:302:VAL:N	1:B:303:PRO:HD2	2.31	0.46
1:A:207:LYS:HA	6:A:1046:HOH:O	2.16	0.45
1:A:268:ALA:C	1:A:269:LEU:HD23	2.41	0.45
1:A:201:LEU:CD1	1:A:221:VAL:HG11	2.46	0.45
1:B:84:SER:OG	1:B:85:ILE:N	2.50	0.45
5:B:2031:TRP:HZ3	6:B:2060:HOH:O	1.99	0.45
1:B:268:ALA:O	1:B:269:LEU:HD23	2.16	0.45
1:A:238:VAL:HG23	6:A:1045:HOH:O	2.17	0.45
1:B:186:MET:HG3	1:B:187:LEU:N	2.30	0.45
1:A:153:LEU:HA	1:A:153:LEU:HD23	1.70	0.45
1:A:88:ILE:HG13	1:A:88:ILE:O	2.17	0.44
1:A:109:ASN:HB3	1:A:110:PRO:HD2	1.98	0.44
1:A:52:ASP:OD1	1:A:52:ASP:C	2.60	0.44
1:B:161:HIS:O	1:B:162:ALA:C	2.60	0.44
1:B:194:SER:C	1:B:196:LYS:H	2.25	0.44
1:A:23:PHE:CE1	1:A:128:MET:HE1	2.52	0.43
1:B:66:LYS:HE3	6:B:2059:HOH:O	2.18	0.43
1:B:66:LYS:O	1:B:68:GLU:N	2.52	0.43
1:A:63:GLU:OE1	1:A:63:GLU:CA	2.58	0.43
1:B:62:VAL:CG1	1:B:68:GLU:HG3	2.49	0.43
1:A:157:SER:C	1:A:159:THR:H	2.26	0.43
1:B:17:ILE:O	1:B:21:VAL:HG23	2.19	0.42
1:B:192:ASN:HB2	6:B:2087:HOH:O	2.18	0.42
1:B:66:LYS:C	1:B:68:GLU:N	2.76	0.42
1:B:283:THR:O	1:B:289:ALA:HB2	2.20	0.42
1:A:44:ASN:OD1	1:A:46:GLU:HB3	2.19	0.42
1:B:228:ASP:HB2	1:B:229:ILE:HD12	2.02	0.42
1:A:154:LEU:CD1	1:A:183:GLY:HA3	2.49	0.42
1:B:12:PRO:HD3	6:B:2074:HOH:O	2.20	0.42
1:B:181:GLU:CG	6:B:2091:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:TYR:O	1:A:53:TYR:CD1	2.73	0.41
1:A:26:LEU:HB2	1:A:129:PHE:CE2	2.55	0.41
1:A:28:LYS:O	1:A:32:GLY:HA2	2.21	0.41
1:B:265:GLU:OE2	1:B:290:PHE:HB2	2.21	0.41
1:A:138:LYS:O	1:A:141:ALA:HB3	2.20	0.41
1:A:268:ALA:O	1:A:269:LEU:HD23	2.21	0.41
1:B:291:LEU:HD12	1:B:291:LEU:HA	1.93	0.41
1:A:47:THR:O	1:A:48:ALA:C	2.62	0.41
1:B:303:PRO:HG2	1:B:304:GLN:OE1	2.21	0.41
1:B:60:ARG:NH2	1:B:68:GLU:OE2	2.47	0.40
1:A:282:PHE:C	1:A:282:PHE:CD1	2.99	0.40
1:B:298:LYS:HE2	4:B:1002:2PN:O1	2.21	0.40
1:A:137:PRO:HD2	1:A:140:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	308/310 (99%)	276 (90%)	30 (10%)	2 (1%)	21	51
1	B	308/310 (99%)	281 (91%)	24 (8%)	3 (1%)	12	38
All	All	616/620 (99%)	557 (90%)	54 (9%)	5 (1%)	16	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	ALA
1	B	192	ASN
1	B	286	ASN
1	A	79	ASN
1	A	202	ILE

5.3.2 Protein sidechains ⓘ

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	256/256 (100%)	231 (90%)	25 (10%)	7	25
1	B	256/256 (100%)	233 (91%)	23 (9%)	9	28
All	All	512/512 (100%)	464 (91%)	48 (9%)	8	27

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	62	VAL
1	A	76	THR
1	A	123	SER
1	A	132	ASN
1	A	136	VAL
1	A	139	GLU
1	A	154	LEU
1	A	160	THR
1	A	169	LYS
1	A	201	LEU
1	A	212	ASN
1	A	217	ARG
1	A	226	ILE
1	A	232	ARG
1	A	235	GLU
1	A	236	ILE
1	A	250	SER
1	A	251	ASP
1	A	264	SER
1	A	269	LEU
1	A	282	PHE
1	A	285	GLU
1	A	291	LEU
1	A	298	LYS
1	B	17	ILE
1	B	42	THR

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Mol	Chain	Res	Type
1	B	71	GLU
1	B	72	THR
1	B	136	VAL
1	B	160	THR
1	B	181	GLU
1	B	184	LEU
1	B	186	MET
1	B	194	SER
1	B	201	LEU
1	B	221	VAL
1	B	224	VAL
1	B	228	ASP
1	B	232	ARG
1	B	234	GLU
1	B	257	THR
1	B	264	SER
1	B	282	PHE
1	B	283	THR
1	B	291	LEU
1	B	298	LYS
1	B	306	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	79	ASN
1	A	132	ASN
1	A	222	ASN
1	A	286	ASN
1	B	222	ASN
1	B	241	GLN
1	B	286	ASN

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 10 ligands modelled in this entry, 6 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$
5	TRP	A	1031	-	15,16,16	1.35	2 (13%)	18,22,22	1.05	1 (5%)
5	TRP	B	2031	-	15,16,16	1.52	5 (33%)	18,22,22	1.11	2 (11%)
4	2PN	B	1002	2,3	8,8,8	2.63	5 (62%)	8,13,13	1.93	3 (37%)
4	2PN	A	1001	2,3	8,8,8	2.63	5 (62%)	8,13,13	2.66	3 (37%)

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
5	TRP	A	1031	-	-	2/8/8/8	0/2/2/2
5	TRP	B	2031	-	-	6/8/8/8	0/2/2/2
4	2PN	B	1002	2,3	-	2/2/6/6	-
4	2PN	A	1001	2,3	-	1/2/6/6	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	2PN	P2-O4	4.74	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1002	2PN	P1-O1	3.98	1.52	1.46
4	B	1002	2PN	P2-O4	3.64	1.51	1.46
4	A	1001	2PN	P2-N1	2.75	1.70	1.63
5	B	2031	TRP	CH2-CZ3	2.63	1.44	1.38
4	A	1001	2PN	P1-O1	2.58	1.50	1.46
4	A	1001	2PN	P1-O2	-2.57	1.50	1.56
4	B	1002	2PN	P2-N1	2.55	1.70	1.63
4	A	1001	2PN	P1-O3	-2.51	1.50	1.56
4	B	1002	2PN	P1-N1	2.48	1.69	1.63
5	B	2031	TRP	CZ3-CE3	2.36	1.42	1.38
5	A	1031	TRP	CD1-CG	2.27	1.40	1.36
5	A	1031	TRP	CD2-CE2	2.27	1.44	1.41
5	B	2031	TRP	CD2-CE2	2.23	1.44	1.41
5	B	2031	TRP	CZ2-CE2	2.15	1.43	1.39
4	B	1002	2PN	P1-O2	-2.11	1.51	1.56
5	B	2031	TRP	CB-CG	2.06	1.54	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	2PN	O4-P2-N1	-5.17	104.16	111.77
4	A	1001	2PN	O1-P1-N1	-4.04	105.81	111.77
4	B	1002	2PN	O1-P1-N1	-3.75	106.25	111.77
5	B	2031	TRP	OXT-C-O	-3.62	115.86	124.08
5	A	1031	TRP	OXT-C-O	-3.42	116.32	124.08
4	B	1002	2PN	O4-P2-N1	-2.85	107.58	111.77
4	A	1001	2PN	O2-P1-O3	2.43	114.11	107.59
5	B	2031	TRP	CA-CB-CG	2.29	117.84	113.49
4	B	1002	2PN	O6-P2-O5	2.11	113.26	107.59

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1002	2PN	P2-N1-P1-O1
4	B	1002	2PN	P1-N1-P2-O4
5	A	1031	TRP	CA-CB-CG-CD2
5	B	2031	TRP	CA-CB-CG-CD2
5	A	1031	TRP	CA-CB-CG-CD1
5	B	2031	TRP	CA-CB-CG-CD1
5	B	2031	TRP	O-C-CA-N
5	B	2031	TRP	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
5	B	2031	TRP	OXT-C-CA-CB
5	B	2031	TRP	O-C-CA-CB
4	A	1001	2PN	P2-N1-P1-O1

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1031	TRP	4	0
5	B	2031	TRP	6	0
4	B	1002	2PN	1	0
4	A	1001	2PN	3	0

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 [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	310/310 (100%)	-0.79	0 100 100	18, 18, 18, 18	0
1	B	310/310 (100%)	-0.77	0 100 100	18, 18, 18, 18	0
All	All	620/620 (100%)	-0.78	0 100 100	18, 18, 18, 18	0

There are no RSRZ outliers to report.

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
5	TRP	A	1031	15/15	0.89	0.12	17,18,18,18	0
5	TRP	B	2031	15/15	0.91	0.13	17,18,18,18	0
3	MG	A	501	1/1	0.92	0.13	17,17,17,17	0
3	MG	B	502	1/1	0.93	0.26	18,18,18,18	0
4	2PN	A	1001	9/9	0.95	0.09	17,18,18,18	0
4	2PN	B	1002	9/9	0.98	0.06	17,18,18,18	0
2	MN	B	403	1/1	0.99	0.02	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	B	404	1/1	0.99	0.01	18,18,18,18	0
2	MN	A	401	1/1	0.99	0.02	17,17,17,17	0
2	MN	A	402	1/1	0.99	0.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.