



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:59 am BST

PDB ID : 1KXJ
Title : The Crystal Structure of Glutamine Amidotransferase from *Thermotoga maritima*
Authors : Korolev, S.; Skarina, T.; Evdokimova, E.; Beasley, S.; Edwards, A.; Joachimiak, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2002-01-31
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

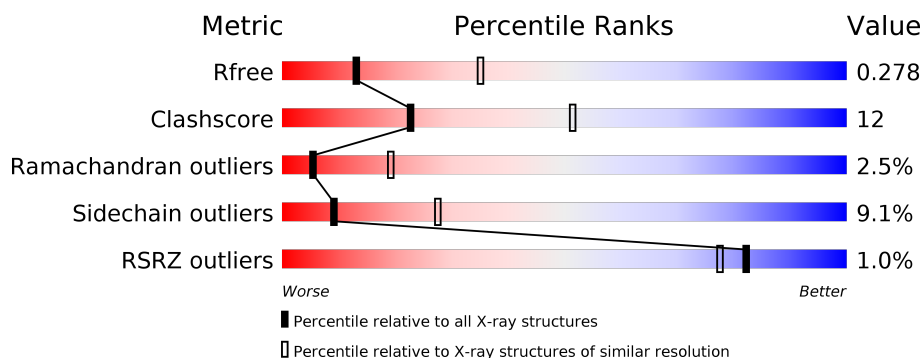
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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	205	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>..</div> </div> </div>
1	B	205	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3282 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 Amidotransferase hisH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1634	1040	289	297	8			
1	B	201	Total	C	N	O	S	0	0	0
			1618	1031	284	295	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q9X0C8
A	0	HIS	-	CLONING ARTIFACT	UNP Q9X0C8
A	202	GLY	-	CLONING ARTIFACT	UNP Q9X0C8
A	203	SER	-	CLONING ARTIFACT	UNP Q9X0C8
B	-1	GLY	-	CLONING ARTIFACT	UNP Q9X0C8
B	0	HIS	-	CLONING ARTIFACT	UNP Q9X0C8
B	202	GLY	-	CLONING ARTIFACT	UNP Q9X0C8
B	203	SER	-	CLONING ARTIFACT	UNP Q9X0C8

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

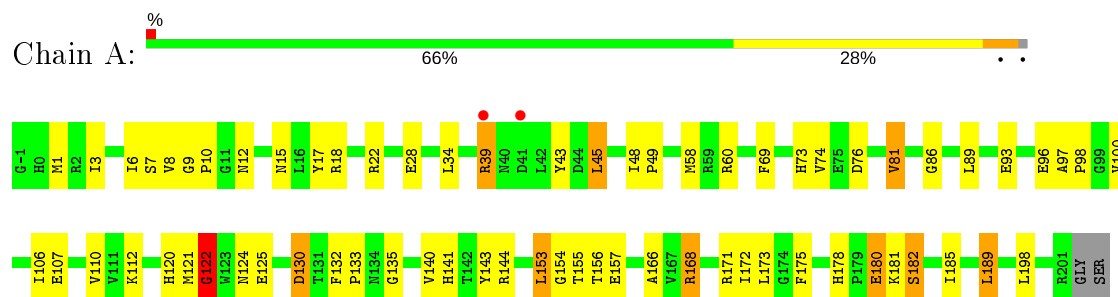


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

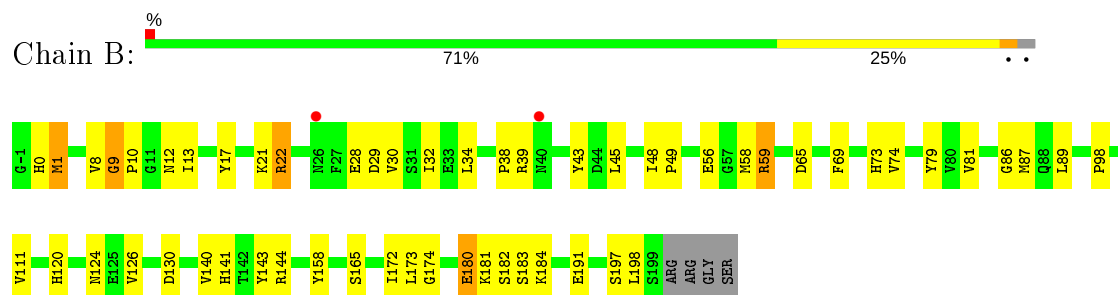
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Amidotransferase hisH



• Molecule 1: Amidotransferase hisH



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.05Å 82.05Å 176.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.96 – 2.80 39.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.6 (39.96-2.80) 97.3 (39.96-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.274 0.234 , 0.278	Depositor DCC
R_{free} test set	1576 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3282	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: PO4

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	0.51	0/1669	0.75	2/2245 (0.1%)
1	B	0.50	0/1653	0.71	0/2224
All	All	0.50	0/3322	0.73	2/4469 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	GLY	N-CA-C	6.13	128.44	113.10
1	A	130	ASP	N-CA-C	5.35	125.45	111.00

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	1634	0	1623	42	0
1	B	1618	0	1608	33	0
2	A	20	0	0	0	0
2	B	10	0	0	0	0
All	All	3282	0	3231	75	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 (75) 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:43:TYR:H	1:A:73:HIS:HE1	1.11	0.97
1:A:43:TYR:H	1:A:73:HIS:CE1	1.91	0.87
1:A:120:HIS:HD1	1:A:141:HIS:HE1	1.19	0.87
1:B:120:HIS:HE2	1:B:124:ASN:ND2	1.76	0.83
1:B:59:ARG:HH11	1:B:59:ARG:HG3	1.44	0.82
1:B:43:TYR:H	1:B:73:HIS:HE1	1.28	0.81
1:A:120:HIS:HD1	1:A:141:HIS:CE1	2.01	0.78
1:B:43:TYR:H	1:B:73:HIS:CE1	2.05	0.74
1:A:120:HIS:ND1	1:A:141:HIS:HE1	1.88	0.71
1:A:1:MET:HE2	1:A:198:LEU:HD23	1.78	0.64
1:A:10:PRO:HD3	1:A:60:ARG:HG3	1.79	0.64
1:B:1:MET:HE2	1:B:198:LEU:HG	1.81	0.62
1:A:69:PHE:O	1:A:73:HIS:HD2	1.82	0.62
1:A:81:VAL:HB	1:A:173:LEU:HB2	1.81	0.61
1:B:69:PHE:O	1:B:73:HIS:HD2	1.83	0.61
1:B:38:PRO:HG3	1:B:65:ASP:O	2.02	0.60
1:B:21:LYS:HA	1:B:32:ILE:CD1	2.33	0.59
1:A:178:HIS:O	1:A:182:SER:HB2	2.02	0.58
1:A:81:VAL:HA	1:A:173:LEU:O	2.05	0.57
1:B:10:PRO:HG3	1:B:56:GLU:HG3	1.87	0.57
1:A:74:VAL:HG13	1:A:172:ILE:HD11	1.88	0.56
1:B:141:HIS:HD2	1:B:143:TYR:O	1.88	0.55
1:A:6:ILE:HG22	1:A:8:VAL:HG12	1.89	0.54
1:B:1:MET:HE2	1:B:198:LEU:CD2	2.38	0.54
1:B:120:HIS:HE2	1:B:124:ASN:HD21	1.55	0.52
1:A:3:ILE:HG23	1:A:45:LEU:HB3	1.91	0.52
1:B:183:SER:OG	1:B:184:LYS:N	2.41	0.52
1:B:48:ILE:O	1:B:86:GLY:HA3	2.10	0.52
1:A:97:ALA:HB1	1:A:100:VAL:HB	1.91	0.52
1:A:180:GLU:O	1:A:181:LYS:HB2	2.09	0.52
1:A:120:HIS:NE2	1:A:124:ASN:ND2	2.59	0.51
1:B:74:VAL:HG22	1:B:172:ILE:HD11	1.92	0.51
1:A:17:TYR:CD1	1:A:34:LEU:HD21	2.47	0.50
1:A:12:ASN:HD21	1:A:15:ASN:ND2	2.10	0.49
1:B:81:VAL:HG22	1:B:173:LEU:HB2	1.95	0.49
1:A:156:THR:HG22	1:A:157:GLU:N	2.27	0.49
1:A:154:GLY:N	1:A:166:ALA:HB3	2.28	0.48
1:A:8:VAL:HG13	1:A:9:GLY:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:HD2	1:A:143:TYR:O	1.97	0.48
1:A:121:MET:O	1:A:122:GLY:O	2.32	0.48
1:B:21:LYS:HA	1:B:32:ILE:HD13	1.96	0.48
1:A:135:GLY:HA3	1:A:185:ILE:CD1	2.43	0.48
1:B:120:HIS:ND1	1:B:141:HIS:HE1	2.12	0.47
1:A:48:ILE:O	1:A:86:GLY:HA3	2.14	0.47
1:A:1:MET:HE2	1:A:198:LEU:CD2	2.43	0.47
1:B:120:HIS:ND1	1:B:141:HIS:CE1	2.83	0.47
1:B:120:HIS:NE2	1:B:124:ASN:ND2	2.56	0.46
1:B:120:HIS:CD2	1:B:158:TYR:CD1	3.04	0.46
1:B:1:MET:HE2	1:B:198:LEU:CG	2.44	0.46
1:B:58:MET:SD	1:B:89:LEU:HD22	2.55	0.46
1:A:112:LYS:HB2	1:A:143:TYR:CE2	2.51	0.45
1:B:79:TYR:CD1	1:B:197:SER:HA	2.52	0.45
1:A:96:GLU:O	1:A:98:PRO:HD3	2.17	0.45
1:B:59:ARG:NH1	1:B:59:ARG:HG3	2.20	0.45
1:B:126:VAL:HG13	1:B:165:SER:OG	2.17	0.44
1:B:180:GLU:O	1:B:181:LYS:HB2	2.18	0.44
1:A:110:VAL:HG12	1:A:143:TYR:HB3	1.99	0.44
1:B:1:MET:HG3	1:B:30:VAL:HG13	1.99	0.43
1:B:87:MET:HG3	1:B:174:GLY:C	2.39	0.43
1:A:7:SER:HB3	1:A:34:LEU:HB3	2.00	0.43
1:A:132:PHE:HA	1:A:133:PRO:HD3	1.84	0.43
1:A:58:MET:SD	1:A:89:LEU:HD22	2.60	0.42
1:B:22:ARG:HB2	1:B:22:ARG:HH11	1.84	0.42
1:A:175:PHE:CE2	1:A:189:LEU:HD11	2.54	0.42
1:A:120:HIS:ND1	1:A:141:HIS:CE1	2.72	0.42
1:A:6:ILE:CG2	1:A:8:VAL:HG12	2.50	0.42
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.83	0.42
1:A:168:ARG:HG3	1:A:173:LEU:CD2	2.49	0.42
1:B:74:VAL:HG22	1:B:172:ILE:CD1	2.50	0.41
1:A:12:ASN:ND2	1:A:15:ASN:ND2	2.69	0.41
1:B:8:VAL:O	1:B:9:GLY:O	2.38	0.41
1:A:168:ARG:HG3	1:A:173:LEU:HD23	2.01	0.41
1:B:17:TYR:CD1	1:B:34:LEU:HD21	2.55	0.40
1:A:132:PHE:CE1	1:A:153:LEU:HD11	2.55	0.40
1:A:107:GLU:HG2	1:A:107:GLU:H	1.76	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	201/205 (98%)	185 (92%)	11 (6%)	5 (2%)	5	19
1	B	199/205 (97%)	185 (93%)	9 (4%)	5 (2%)	5	19
All	All	400/410 (98%)	370 (92%)	20 (5%)	10 (2%)	5	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLY
1	A	140	VAL
1	B	9	GLY
1	B	130	ASP
1	B	140	VAL
1	A	39	ARG
1	A	130	ASP
1	B	49	PRO
1	B	98	PRO
1	A	49	PRO

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	177/179 (99%)	160 (90%)	17 (10%)	8	24
1	B	176/179 (98%)	161 (92%)	15 (8%)	10	31
All	All	353/358 (99%)	321 (91%)	32 (9%)	9	27

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	28	GLU
1	A	39	ARG
1	A	45	LEU
1	A	76	ASP
1	A	81	VAL
1	A	93	GLU
1	A	106	ILE
1	A	125	GLU
1	A	144	ARG
1	A	153	LEU
1	A	155	THR
1	A	168	ARG
1	A	171	ARG
1	A	180	GLU
1	A	182	SER
1	A	189	LEU
1	B	0	HIS
1	B	1	MET
1	B	12	ASN
1	B	13	ILE
1	B	22	ARG
1	B	28	GLU
1	B	29	ASP
1	B	39	ARG
1	B	45	LEU
1	B	59	ARG
1	B	111	VAL
1	B	144	ARG
1	B	180	GLU
1	B	182	SER
1	B	191	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	64	ASN
1	A	73	HIS
1	A	109	ASN
1	A	124	ASN

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Mol	Chain	Res	Type
1	A	141	HIS
1	B	64	ASN
1	B	73	HIS
1	B	124	ASN
1	B	141	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are 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	$\# Z > 2$
2	PO4	B	205	-	4,4,4	1.68	1 (25%)	6,6,6	0.42	0
2	PO4	A	205	-	4,4,4	1.39	0	6,6,6	0.49	0
2	PO4	A	204	-	4,4,4	1.56	0	6,6,6	0.43	0
2	PO4	A	207	-	4,4,4	0.42	0	6,6,6	0.49	0
2	PO4	B	204	-	4,4,4	1.42	0	6,6,6	0.43	0
2	PO4	A	206	-	4,4,4	1.57	0	6,6,6	0.41	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	205	PO4	P-O4	-2.04	1.48	1.54

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 [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	203/205 (99%)	-0.33	2 (0%) 82 77	15, 33, 63, 76	0
1	B	201/205 (98%)	-0.33	2 (0%) 82 77	14, 34, 66, 76	0
All	All	404/410 (98%)	-0.33	4 (0%) 82 77	14, 34, 65, 76	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	40	ASN	2.9
1	B	26	ASN	2.6
1	A	41	ASP	2.3
1	A	39	ARG	2.1

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 carbohydrates 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	PO4	B	204	5/5	0.93	0.26	69,70,71,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	A	206	5/5	0.93	0.13	66,67,68,68	0
2	PO4	A	204	5/5	0.94	0.26	57,58,62,62	0
2	PO4	A	207	5/5	0.94	0.15	64,66,66,68	0
2	PO4	B	205	5/5	0.94	0.14	58,59,60,60	0
2	PO4	A	205	5/5	0.94	0.18	61,64,64,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.