



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2024 – 01:04 PM EDT

PDB ID : 8W05  
Title : Crystal Structure of the reconstruction of the ancestral triosephosphate isomerase of the last opisthokont common ancestor obtained by maximum likelihood  
Authors : Perez-Nino, J.A.; Rodriguez-Romero, A.; Guerra-Borrego, Y.; Fernandez-Velasco, D.A.  
Deposited on : 2024-02-13  
Resolution : 2.16 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.002 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.3

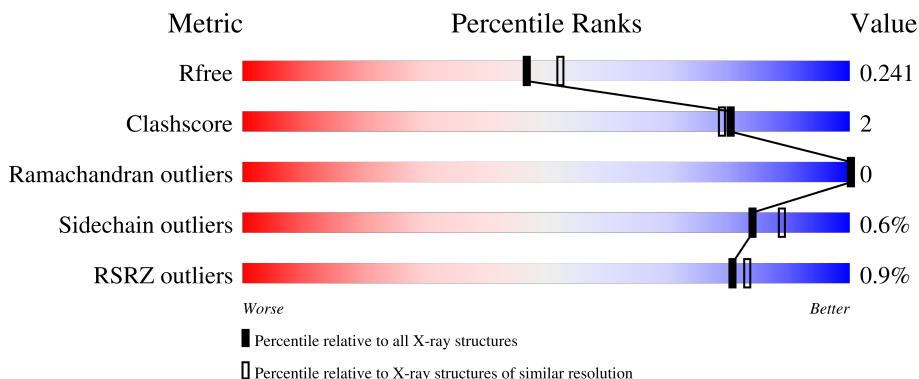
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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))
$R_{free}$	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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  $\geq 3$ , 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	270	 88% 8%
1	B	270	 87% 6% 7%
1	C	270	 87% 8%
1	D	270	 84% 7% 9%
1	E	270	 84% 8% 8%

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Mol	Chain	Length	Quality of chain
1	F	270	 87% 8%
1	G	270	 84% 8% 8%
1	H	270	 84% 8% 8%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 16455 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 Triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	249	Total 1919	C 1212	N 327	O 374	S 6	0	1	0
1	B	252	Total 1946	C 1228	N 332	O 379	S 7	0	1	0
1	C	248	Total 1910	C 1207	N 326	O 371	S 6	0	1	0
1	D	246	Total 1911	C 1209	N 325	O 369	S 8	0	1	0
1	E	249	Total 1915	C 1211	N 327	O 370	S 7	0	1	0
1	F	248	Total 1921	C 1213	N 327	O 375	S 6	0	2	0
1	G	249	Total 1913	C 1210	N 326	O 370	S 7	0	0	0
1	H	249	Total 1889	C 1196	N 324	O 362	S 7	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	208	Total 208	O 208	0	0
2	B	174	Total 174	O 174	0	0
2	C	151	Total 151	O 151	0	0
2	D	145	Total 145	O 145	0	0
2	E	117	Total 117	O 117	0	0
2	F	129	Total 129	O 129	0	0

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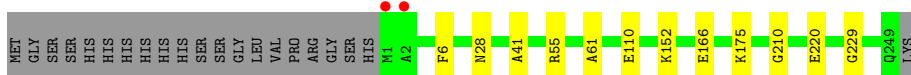
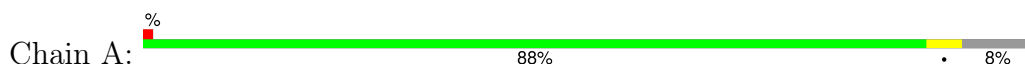
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	G	121	Total 121	O 121	0	0
2	H	86	Total 86	O 86	0	0

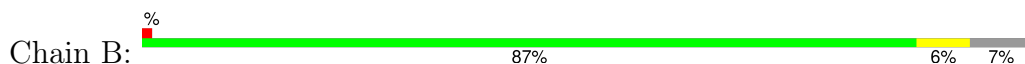
### 3 Residue-property plots [i](#)

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.

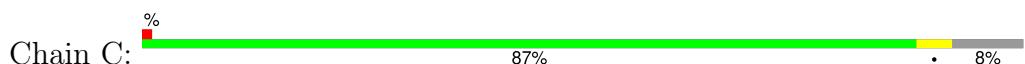
- Molecule 1: Triosephosphate isomerase



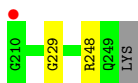
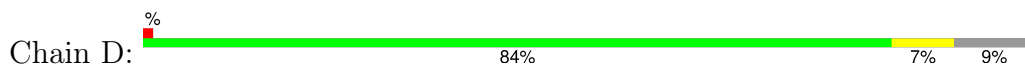
- Molecule 1: Triosephosphate isomerase



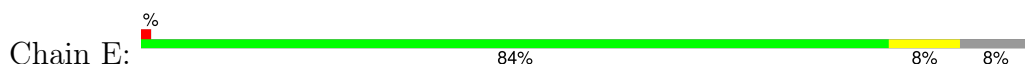
- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase

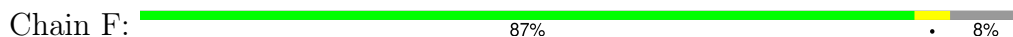


- Molecule 1: Triosephosphate isomerase

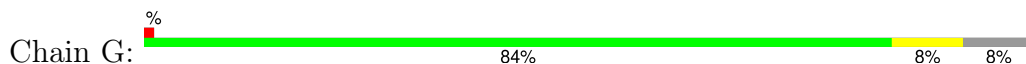




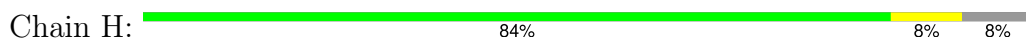
● Molecule 1: Triosephosphate isomerase



● Molecule 1: Triosephosphate isomerase



● Molecule 1: Triosephosphate isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.42Å 83.60Å 126.02Å 90.00° 105.77° 90.00°	Depositor
Resolution (Å)	43.80 – 2.16 43.80 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.80-2.16) 98.2 (43.80-2.17)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.16Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.190 , 0.240 0.190 , 0.241	Depositor DCC
$R_{free}$ test set	5755 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.47	0/1950	0.61	0/2641
1	B	0.47	0/1978	0.62	0/2676
1	C	0.46	0/1941	0.64	0/2629
1	D	0.47	0/1942	0.60	0/2627
1	E	0.38	0/1946	0.58	0/2634
1	F	0.42	0/1952	0.58	0/2642
1	G	0.42	0/1944	0.56	0/2631
1	H	0.41	0/1920	0.59	0/2603
All	All	0.44	0/15573	0.60	0/21083

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	206	ARG	Sidechain

### 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	1919	0	1919	7	0
1	B	1946	0	1950	9	0
1	C	1910	0	1910	7	0
1	D	1911	0	1918	10	0
1	E	1915	0	1926	13	0
1	F	1921	0	1926	7	0
1	G	1913	0	1926	12	0
1	H	1889	0	1888	11	0
2	A	208	0	0	2	0
2	B	174	0	0	1	0
2	C	151	0	0	0	0
2	D	145	0	0	1	0
2	E	117	0	0	0	0
2	F	129	0	0	2	0
2	G	121	0	0	0	0
2	H	86	0	0	0	0
All	All	16455	0	15363	76	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 (76) 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:126:ILE:HD12	1:B:142:VAL:HG13	1.63	0.79
1:A:220:GLU:HG2	2:A:401:HOH:O	1.87	0.73
1:H:126:ILE:HD12	1:H:142:VAL:HG13	1.74	0.68
1:E:1:MET:HG3	1:E:2:ALA:H	1.61	0.66
1:C:28:ASN:HA	1:C:55:ARG:HD2	1.81	0.61
1:G:191:LYS:O	1:G:195:GLU:HG3	2.01	0.60
1:A:28:ASN:HA	1:A:55:ARG:HD2	1.84	0.60
1:D:153:ILE:HD11	1:D:158:TRP:CE2	2.37	0.59
1:B:6:PHE:O	1:B:229:GLY:HA3	2.04	0.58
1:C:166:GLU:HB3	1:C:171:ILE:HD11	1.86	0.56
1:H:48:PRO:HG3	1:H:85:LEU:HD21	1.87	0.56
1:H:177:ALA:HB1	1:H:181:GLN:HG3	1.86	0.56
1:B:28:ASN:HA	1:B:55:ARG:HD2	1.89	0.55
1:D:178:THR:HG23	1:D:181:GLN:OE1	2.07	0.55
1:E:1:MET:CG	1:E:2:ALA:H	2.16	0.55
1:H:6:PHE:O	1:H:229:GLY:HA3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:HG2	1:B:210:GLY:HA3	1.90	0.54
1:C:6:PHE:O	1:C:229:GLY:HA3	2.08	0.53
1:G:177:ALA:HB1	1:G:181:GLN:HG3	1.89	0.53
1:H:42:PRO:HG2	1:H:47:LEU:HD23	1.92	0.51
1:H:28:ASN:HA	1:H:55:ARG:HD2	1.93	0.51
1:G:33:ASP:OD2	1:G:249:GLN:HB2	2.11	0.50
1:H:214:ASN:HB2	1:H:240:GLU:OE2	2.10	0.50
1:G:16:THR:O	1:G:20:ILE:HG13	2.12	0.50
1:E:146:LEU:HD11	1:E:189:ILE:HG23	1.93	0.49
1:G:28:ASN:HA	1:G:55:ARG:HD2	1.93	0.49
1:C:32:LEU:HD23	1:C:242:VAL:HG13	1.94	0.49
1:E:1:MET:HG3	1:E:2:ALA:N	2.27	0.48
1:D:6:PHE:O	1:D:229:GLY:HA3	2.13	0.48
1:B:165:TYR:CE2	1:B:167:PRO:HG3	2.49	0.48
1:A:166:GLU:HG2	1:A:210:GLY:HA3	1.97	0.47
1:A:110:GLU:HG3	1:A:152:LYS:HE3	1.98	0.46
1:F:209:TYR:O	1:F:230:PHE:HA	2.16	0.45
1:G:6:PHE:O	1:G:229:GLY:HA3	2.16	0.45
1:E:28:ASN:HA	1:E:55:ARG:HD2	1.97	0.45
1:G:5:PHE:CE1	1:G:229:GLY:HA2	2.50	0.45
1:E:105:ASP:OD2	1:E:144:ARG:HD2	2.17	0.45
1:B:110:GLU:HG3	1:B:152:LYS:HE3	1.99	0.44
1:E:5:PHE:CE1	1:E:229:GLY:HA2	2.52	0.44
1:C:166:GLU:HG2	1:C:210:GLY:HA3	1.99	0.44
1:D:25:GLU:OE2	1:D:29:ASN:ND2	2.51	0.44
1:E:66:TYR:CE2	1:E:68:LYS:HG3	2.53	0.44
1:H:60:VAL:O	1:H:88:PRO:HD2	2.18	0.44
1:A:175:LYS:HE3	2:A:479:HOH:O	2.18	0.43
1:D:59:GLN:HG2	2:D:431:HOH:O	2.18	0.43
1:F:147:LYS:HG3	1:F:192:TRP:HZ2	1.83	0.43
1:H:36:THR:HG21	1:H:245:ILE:HG23	2.00	0.43
1:D:28:ASN:HA	1:D:55:ARG:HD2	1.99	0.43
1:E:165:TYR:CE1	1:E:185:VAL:HG11	2.52	0.43
1:F:238:LYS:HB3	1:F:239:PRO:HD2	2.00	0.43
1:G:209:TYR:O	1:G:230:PHE:HA	2.18	0.43
1:B:165:TYR:CZ	1:B:167:PRO:HG3	2.54	0.43
1:E:248:ARG:HG3	1:E:248:ARG:NH1	2.33	0.43
1:E:6:PHE:O	1:E:229:GLY:HA3	2.18	0.43
1:B:113:LYS:HE2	2:B:302:HOH:O	2.18	0.43
1:D:8:GLY:HA2	1:D:39:VAL:O	2.19	0.43
1:B:238:LYS:HB3	1:B:239:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:VAL:O	1:D:88:PRO:HD2	2.19	0.42
1:H:11:TRP:CZ3	1:H:42:PRO:HB3	2.54	0.42
1:G:41:ALA:HA	1:G:61:ALA:O	2.19	0.42
1:G:116:LEU:HD13	1:G:157:ASP:HB3	2.02	0.42
1:A:41:ALA:HA	1:A:61:ALA:O	2.20	0.42
1:E:191:LYS:O	1:E:195:GLU:HG3	2.20	0.41
1:G:246:ASN:O	1:G:249:GLN:HB3	2.20	0.41
1:F:116:LEU:HD13	1:F:157:ASP:HB3	2.01	0.41
1:H:139:MET:HA	1:H:139:MET:HE3	2.03	0.41
1:C:200:GLU:H	1:C:200:GLU:CD	2.24	0.41
1:F:179:PRO:HD3	2:F:347:HOH:O	2.19	0.41
1:A:6:PHE:O	1:A:229:GLY:HA3	2.21	0.41
1:C:179:PRO:HA	1:C:221:LEU:HD23	2.02	0.41
1:D:66:TYR:CG	1:D:67:THR:N	2.88	0.41
1:D:109:ALA:HB1	1:D:152:LYS:HD2	2.02	0.41
1:F:28:ASN:HA	1:F:55:ARG:HD2	2.03	0.41
1:F:86:GLY:HA2	2:F:343:HOH:O	2.20	0.40
1:E:41:ALA:HA	1:E:61:ALA:O	2.22	0.40
1:G:20:ILE:HD12	1:G:46:TYR:CG	2.56	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	248/270 (92%)	242 (98%)	6 (2%)	0	100	100
1	B	251/270 (93%)	243 (97%)	8 (3%)	0	100	100
1	C	247/270 (92%)	240 (97%)	7 (3%)	0	100	100
1	D	243/270 (90%)	236 (97%)	7 (3%)	0	100	100
1	E	248/270 (92%)	242 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	248/270 (92%)	241 (97%)	7 (3%)	0	100	100
1	G	247/270 (92%)	239 (97%)	8 (3%)	0	100	100
1	H	247/270 (92%)	237 (96%)	10 (4%)	0	100	100
All	All	1979/2160 (92%)	1920 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	203/222 (91%)	203 (100%)	0	100	100
1	B	207/222 (93%)	206 (100%)	1 (0%)	86	91
1	C	202/222 (91%)	201 (100%)	1 (0%)	86	91
1	D	204/222 (92%)	203 (100%)	1 (0%)	86	91
1	E	203/222 (91%)	202 (100%)	1 (0%)	86	91
1	F	205/222 (92%)	205 (100%)	0	100	100
1	G	203/222 (91%)	202 (100%)	1 (0%)	86	91
1	H	197/222 (89%)	193 (98%)	4 (2%)	50	55
All	All	1624/1776 (91%)	1615 (99%)	9 (1%)	84	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	GLU
1	C	206	ARG
1	D	248	ARG
1	E	155	GLU
1	G	52	GLN
1	H	85	LEU
1	H	140	ASP
1	H	156	SER

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Mol	Chain	Res	Type
1	H	206	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	249/270 (92%)	-0.36	2 (0%) 82 84	12, 25, 38, 53	1 (0%)
1	B	252/270 (93%)	-0.26	2 (0%) 82 84	16, 28, 42, 60	1 (0%)
1	C	248/270 (91%)	-0.13	3 (1%) 76 79	14, 28, 49, 58	1 (0%)
1	D	246/270 (91%)	-0.14	3 (1%) 76 79	17, 29, 46, 67	1 (0%)
1	E	249/270 (92%)	0.03	4 (1%) 70 73	17, 34, 51, 66	1 (0%)
1	F	248/270 (91%)	-0.09	1 (0%) 89 90	16, 32, 47, 54	2 (0%)
1	G	249/270 (92%)	0.04	2 (0%) 82 84	23, 34, 50, 65	0
1	H	249/270 (92%)	0.20	1 (0%) 89 90	24, 37, 53, 69	0
All	All	1990/2160 (92%)	-0.09	18 (0%) 81 83	12, 31, 49, 69	7 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	176	VAL	4.0
1	H	1	MET	3.4
1	E	1	MET	3.3
1	A	1	MET	3.2
1	A	2	ALA	3.1
1	E	2	ALA	3.0
1	G	1	MET	2.9
1	D	171	ILE	2.7
1	G	2	ALA	2.6
1	F	139	MET	2.5
1	C	172	GLY	2.5
1	E	176	VAL	2.5
1	B	-2	GLY	2.5
1	B	249	GLN	2.3
1	C	177	ALA	2.3
1	C	249	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	139	MET	2.1
1	D	210	GLY	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.