Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 12:58 AM JST

PDB ID	:	7E77
Title	:	The structure of cytosolic TaPGI
Authors	:	Gao, F.; Liu, C.M.
Deposited on	:	2021-02-25
Resolution	:	2.04 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:

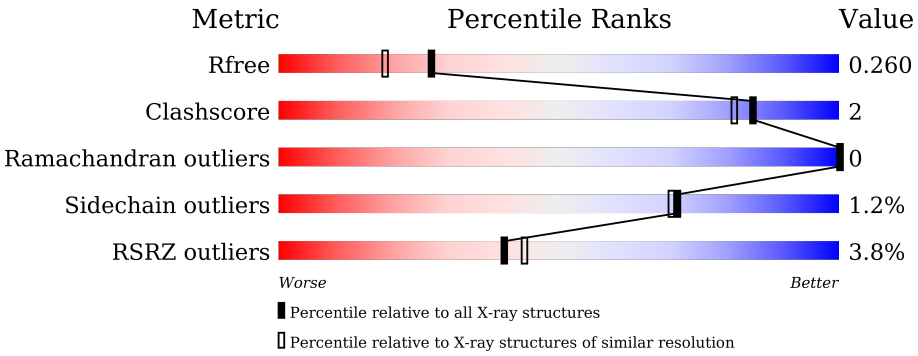
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 <=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	567	2% 93% 6%
1	B	567	3% 90% 6%
1	C	567	5% 93% 7%
1	D	567	4% 90% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17830 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 Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4362	2791	745	815	11			
1	B	549	Total	C	N	O	S	0	0	0
			4265	2728	731	795	11			
1	C	562	Total	C	N	O	S	0	0	0
			4360	2790	744	815	11			
1	D	549	Total	C	N	O	S	0	0	0
			4265	2728	731	795	11			

- Molecule 2 is water.

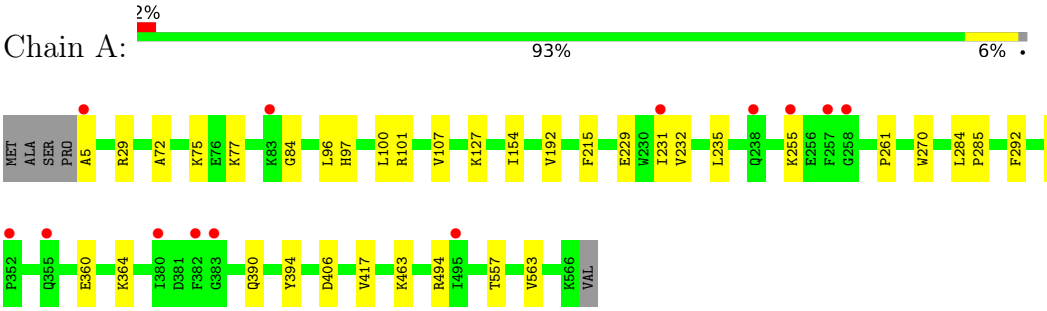
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	136	Total	O	0	0
			136	136		
2	B	127	Total	O	0	0
			127	127		
2	C	146	Total	O	0	0
			146	146		
2	D	169	Total	O	0	0
			169	169		

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.

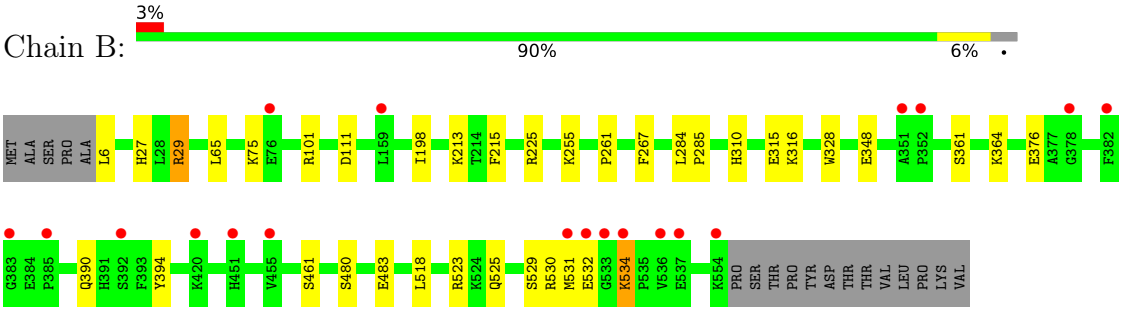
• Molecule 1: Glucose-6-phosphate isomerase

Chain A:



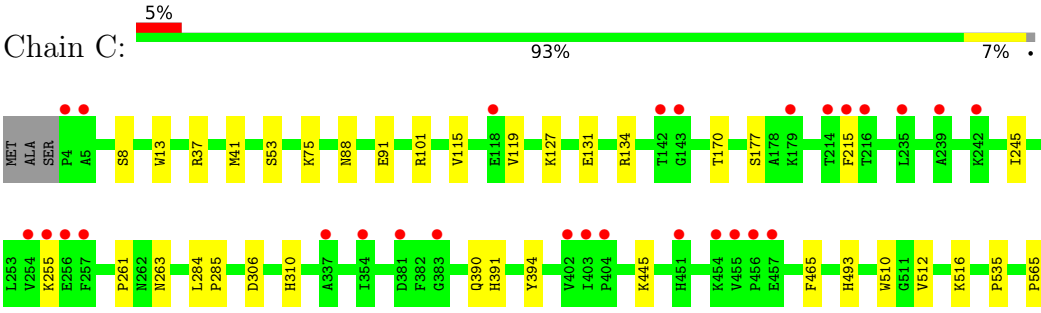
• Molecule 1: Glucose-6-phosphate isomerase

Chain B:



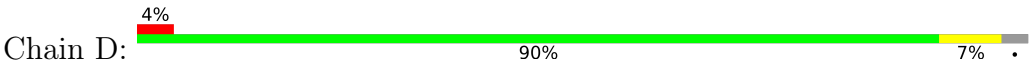
• Molecule 1: Glucose-6-phosphate isomerase

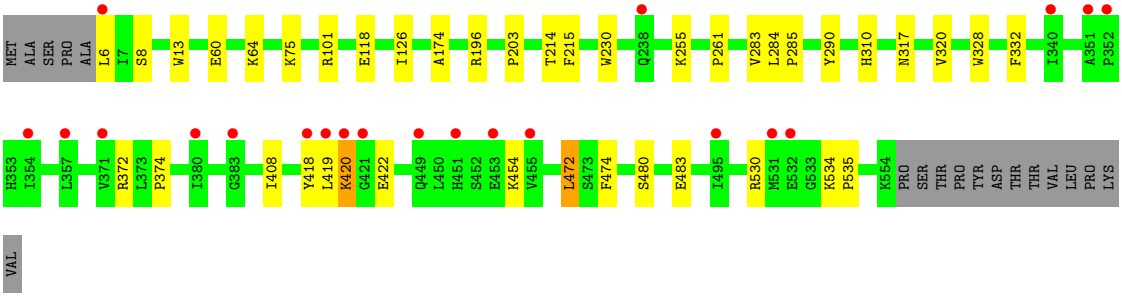
Chain C:



• Molecule 1: Glucose-6-phosphate isomerase

Chain D:




MET ALA SER PRO ALA L6 I7 S8 W13 E60 K64 K75 R101 E118 I126 A174 R196 P203 T214 F215 W230 Q238 K255 P261 V283 L284 P285 Y290 H310 N317 V320 W328 F332 I340 A351 P352
H353 I354 L357 V371 R372 L373 P374 I380 G383 I408 Y418 L419 K420 G421 E422 Q449 L450 H451 S452 E453 K454 V455 L472 S473 F474 S480 E483 I495 R530 M531 E532 G533 K534 P535 K554 PRO SER THR PRO TYR ASP THR THR VAL LEU PRO LYS
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	244.32Å 74.90Å 125.34Å 90.00° 93.80° 90.00°	Depositor
Resolution (Å)	37.91 – 2.04 37.91 – 2.04	Depositor EDS
% Data completeness (in resolution range)	91.5 (37.91-2.04) 91.5 (37.91-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.28 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.254 , 0.260 0.254 , 0.260	Depositor DCC
R_{free} test set	2004 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17830	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.25	0/4464	0.42	0/6060
1	B	0.25	0/4363	0.41	0/5918
1	C	0.24	0/4463	0.41	0/6060
1	D	0.25	0/4363	0.42	0/5918
All	All	0.25	0/17653	0.42	0/23956

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	4362	0	4367	19	0
1	B	4265	0	4269	21	0
1	C	4360	0	4362	21	0
1	D	4265	0	4269	23	0
2	A	136	0	0	1	0
2	B	127	0	0	5	0
2	C	146	0	0	2	0
2	D	169	0	0	2	0
All	All	17830	0	17267	78	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 (78) 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:C:37:ARG:HG2	1:C:41:MET:HE1	1.69	0.75
1:B:529:SER:HA	1:B:534:LYS:H	1.51	0.74
1:C:134:ARG:NH2	1:C:177:SER:O	2.22	0.73
1:D:418:TYR:HE1	1:D:420:LYS:HG3	1.62	0.65
1:D:75:LYS:NZ	1:D:310:HIS:O	2.31	0.64
1:A:557:THR:HG21	1:A:563:VAL:HG11	1.81	0.62
1:D:6:LEU:N	2:D:603:HOH:O	2.33	0.61
1:A:84:GLY:HA2	1:A:96:LEU:HD21	1.83	0.61
1:B:255:LYS:HB2	1:B:261:PRO:HG3	1.82	0.61
1:A:97:HIS:HA	1:A:100:LEU:HD23	1.84	0.60
1:D:418:TYR:CE1	1:D:420:LYS:HG3	2.37	0.59
1:B:6:LEU:N	2:B:608:HOH:O	2.35	0.59
1:A:72:ALA:O	1:A:77:LYS:NZ	2.36	0.59
1:B:65:LEU:HD11	1:B:328:TRP:HB2	1.83	0.58
1:D:255:LYS:HB2	1:D:261:PRO:HG3	1.86	0.56
1:C:252:LYS:NZ	2:C:603:HOH:O	2.30	0.55
1:D:472:LEU:HD11	1:D:474:PHE:CE2	2.41	0.55
1:B:361:SER:O	1:B:364:LYS:NZ	2.39	0.55
1:C:245:ILE:HG22	1:C:263:ASN:HB3	1.88	0.55
1:B:348:GLU:OE1	1:D:196:ARG:NH2	2.41	0.53
1:C:41:MET:HE3	1:C:53:SER:HA	1.91	0.52
1:C:75:LYS:NZ	1:C:310:HIS:O	2.42	0.52
1:C:127:LYS:NZ	1:C:131:GLU:OE2	2.32	0.52
1:A:75:LYS:NZ	1:A:310:HIS:O	2.42	0.52
1:D:408:ILE:HG12	1:D:474:PHE:CD2	2.45	0.51
1:B:213:LYS:HB2	1:B:267:PHE:CZ	2.47	0.49
1:A:255:LYS:HB2	1:A:261:PRO:HG3	1.94	0.48
1:D:60:GLU:HG2	1:D:64:LYS:HE2	1.96	0.48
1:D:408:ILE:HG12	1:D:474:PHE:HD2	1.77	0.48
1:D:480:SER:OG	1:D:483:GLU:OE1	2.30	0.48
1:A:154:ILE:HD12	1:C:391:HIS:CD2	2.49	0.47
1:B:376:GLU:O	2:B:601:HOH:O	2.20	0.47
1:C:8:SER:HA	1:C:13:TRP:CG	2.50	0.47
1:C:535:PRO:O	2:C:601:HOH:O	2.20	0.47
1:C:255:LYS:HB2	1:C:261:PRO:HG3	1.97	0.46
1:A:5:ALA:N	2:A:616:HOH:O	2.47	0.46
1:B:27:HIS:ND1	1:B:29:ARG:HG2	2.30	0.46
1:A:406:ASP:OD2	1:A:494:ARG:NH1	2.33	0.46
1:C:306:ASP:OD1	1:C:493:HIS:NE2	2.41	0.46
1:B:530:ARG:NH2	2:B:610:HOH:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG23	1:A:235:LEU:HD12	1.96	0.46
1:A:390:GLN:HA	1:A:394:TYR:CG	2.50	0.46
1:D:328:TRP:HA	1:D:332:PHE:HD2	1.80	0.46
1:B:523:ARG:NH1	2:B:605:HOH:O	2.32	0.46
1:D:419:LEU:HD23	1:D:419:LEU:HA	1.86	0.45
1:A:229:GLU:HA	1:A:232:VAL:HG22	1.98	0.45
1:A:284:LEU:HB3	1:A:285:PRO:HD3	1.98	0.45
1:A:360:GLU:O	1:A:364:LYS:NZ	2.51	0.44
1:D:126:ILE:HG21	1:D:283:VAL:HG12	1.99	0.44
1:A:417:VAL:HG22	1:C:565:PRO:HD3	1.99	0.44
1:B:480:SER:OG	1:B:483:GLU:OE1	2.25	0.44
1:D:317:ASN:HB3	1:D:320:VAL:HB	1.99	0.44
1:B:198:ILE:O	2:B:602:HOH:O	2.21	0.44
1:C:88:ASN:ND2	1:C:91:GLU:OE1	2.47	0.43
1:B:284:LEU:HB3	1:B:285:PRO:HD3	2.00	0.43
1:B:390:GLN:HA	1:B:394:TYR:CG	2.54	0.43
1:C:390:GLN:HA	1:C:394:TYR:CG	2.54	0.43
1:D:203:PRO:HG3	1:D:230:TRP:CE2	2.54	0.42
1:A:127:LYS:HD3	1:A:292:PHE:CD2	2.54	0.42
1:C:512:VAL:HG22	1:C:516:LYS:HE3	2.01	0.42
1:A:192:VAL:HG13	1:C:170:THR:HG21	2.01	0.42
1:B:525:GLN:NE2	1:B:529:SER:OG	2.50	0.42
1:C:445:LYS:H	1:C:465:PHE:HB2	1.85	0.42
1:C:284:LEU:HB3	1:C:285:PRO:HD3	2.01	0.42
1:D:214:THR:HA	2:D:650:HOH:O	2.19	0.42
1:B:75:LYS:NZ	1:B:310:HIS:O	2.53	0.41
1:D:174:ALA:HB1	1:D:290:TYR:CD1	2.55	0.41
1:B:315:GLU:OE2	1:B:316:LYS:NZ	2.54	0.41
1:D:8:SER:HA	1:D:13:TRP:CG	2.56	0.41
1:D:534:LYS:HG2	1:D:535:PRO:HD2	2.02	0.41
1:B:532:GLU:H	1:B:532:GLU:HG3	1.69	0.41
1:B:225:ARG:NE	1:D:422:GLU:OE2	2.50	0.41
1:A:96:LEU:HB2	1:A:270:TRP:CE3	2.56	0.41
1:B:6:LEU:HD12	1:B:6:LEU:HA	1.84	0.41
1:A:463:LYS:HE2	1:C:510:TRP:CZ3	2.56	0.40
1:C:115:VAL:O	1:C:119:VAL:HG23	2.20	0.40
1:D:6:LEU:HD21	1:D:374:PRO:HD3	2.04	0.40
1:D:284:LEU:HB3	1:D:285:PRO:HD3	2.03	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	560/567 (99%)	552 (99%)	8 (1%)	0	100	100
1	B	547/567 (96%)	536 (98%)	11 (2%)	0	100	100
1	C	560/567 (99%)	549 (98%)	11 (2%)	0	100	100
1	D	547/567 (96%)	535 (98%)	12 (2%)	0	100	100
All	All	2214/2268 (98%)	2172 (98%)	42 (2%)	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	477/481 (99%)	473 (99%)	4 (1%)	81	82
1	B	465/481 (97%)	457 (98%)	8 (2%)	60	57
1	C	477/481 (99%)	475 (100%)	2 (0%)	91	91
1	D	465/481 (97%)	457 (98%)	8 (2%)	60	57
All	All	1884/1924 (98%)	1862 (99%)	22 (1%)	71	70

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	101	ARG

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Mol	Chain	Res	Type
1	A	107	VAL
1	A	215	PHE
1	B	29	ARG
1	B	101	ARG
1	B	111	ASP
1	B	215	PHE
1	B	461	SER
1	B	518	LEU
1	B	531	MET
1	B	534	LYS
1	C	101	ARG
1	C	215	PHE
1	D	101	ARG
1	D	118	GLU
1	D	215	PHE
1	D	372	ARG
1	D	420	LYS
1	D	454	LYS
1	D	472	LEU
1	D	530	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 monosaccharides 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^{th} 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	562/567 (99%)	0.29	14 (2%)	57	61	38, 59, 88, 114	0
1	B	549/567 (96%)	0.27	19 (3%)	44	48	41, 59, 82, 177	0
1	C	562/567 (99%)	0.39	30 (5%)	26	28	39, 59, 90, 113	0
1	D	549/567 (96%)	0.28	21 (3%)	40	44	35, 53, 83, 125	0
All	All	2222/2268 (97%)	0.31	84 (3%)	40	44	35, 57, 87, 177	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	531	MET	7.1
1	C	248	SER	7.0
1	C	4	PRO	5.3
1	B	534	LYS	4.6
1	D	421	GLY	4.5
1	D	451	HIS	4.4
1	D	418	TYR	4.3
1	D	419	LEU	4.2
1	C	235	LEU	4.0
1	C	242	LYS	3.9
1	B	159	LEU	3.8
1	C	257	PHE	3.5
1	C	455	VAL	3.3
1	B	532	GLU	3.2
1	D	532	GLU	3.2
1	C	254	VAL	3.1
1	C	179	LYS	3.0
1	B	420	LYS	3.0
1	D	531	MET	3.0
1	C	354	ILE	3.0
1	A	383	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	5	ALA	2.9
1	C	215	PHE	2.9
1	D	449	GLN	2.9
1	D	455	VAL	2.9
1	A	258	GLY	2.9
1	C	239	ALA	2.9
1	C	256	GLU	2.8
1	C	383	GLY	2.7
1	C	451	HIS	2.7
1	A	380	ILE	2.7
1	C	118	GLU	2.7
1	C	255	LYS	2.7
1	A	337	ALA	2.7
1	B	537	GLU	2.6
1	C	404	PRO	2.6
1	D	380	ILE	2.6
1	B	451	HIS	2.6
1	B	536	VAL	2.6
1	B	392	SER	2.6
1	B	554	LYS	2.6
1	D	420	LYS	2.6
1	D	340	ILE	2.5
1	B	382	PHE	2.5
1	D	238	GLN	2.5
1	C	403	ILE	2.5
1	D	453	GLU	2.5
1	A	257	PHE	2.5
1	C	214	THR	2.5
1	B	383	GLY	2.5
1	B	351	ALA	2.5
1	C	454	LYS	2.5
1	A	382	PHE	2.4
1	B	455	VAL	2.4
1	A	352	PRO	2.4
1	A	355	GLN	2.4
1	C	402	VAL	2.4
1	C	381	ASP	2.3
1	C	251	LEU	2.3
1	B	385	PRO	2.3
1	C	142	THR	2.3
1	A	495	ILE	2.3
1	D	6	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	76	GLU	2.3
1	A	231	ILE	2.2
1	D	351	ALA	2.2
1	B	352	PRO	2.2
1	C	457	GLU	2.2
1	D	357	LEU	2.2
1	A	238	GLN	2.2
1	D	383	GLY	2.2
1	C	5	ALA	2.1
1	C	143	GLY	2.1
1	C	456	PRO	2.1
1	C	337	ALA	2.1
1	A	255	LYS	2.1
1	B	378	GLY	2.1
1	D	354	ILE	2.1
1	C	216	THR	2.1
1	D	495	ILE	2.0
1	D	352	PRO	2.0
1	D	371	VAL	2.0
1	A	83	LYS	2.0
1	B	533	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.