



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2022 – 01:16 pm BST

PDB ID : 7PEJ
Title : Crystal structure of Triosephosphate Isomerase from Schizosaccharomyces pombe (SpTIM wt)
Authors : Romero-Romero, S.; Garza-Ramos, G.
Deposited on : 2021-08-10
Resolution : 1.79 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
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

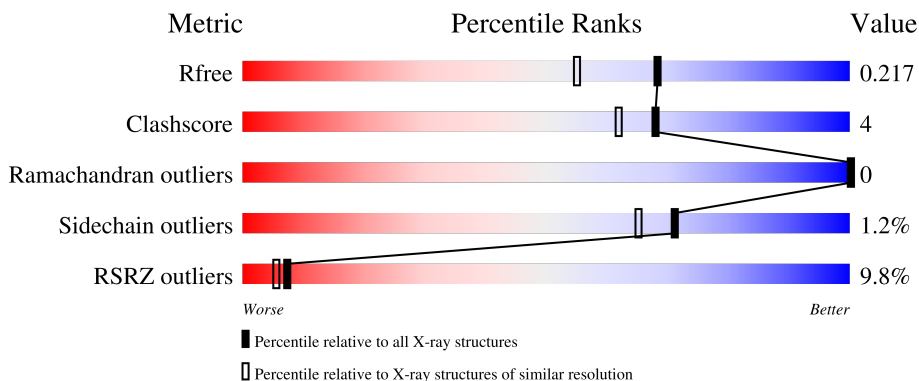
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

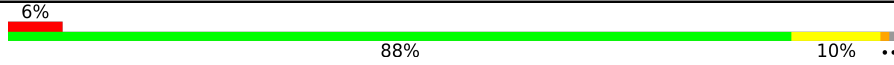
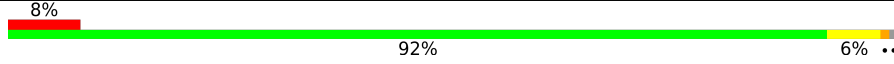
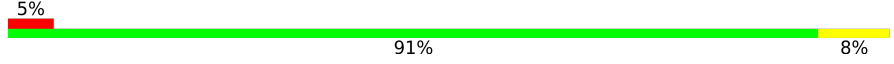
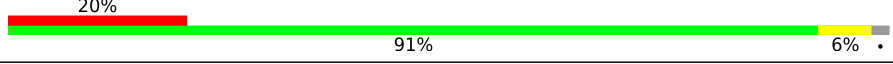
The reported resolution of this entry is 1.79 Å.

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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	248	 6% 88% 10% ..
1	B	248	 8% 92% 6% ..
1	C	248	 5% 91% 8% ..
1	D	248	 20% 91% 6% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8277 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	246	1871	1183	322	361	5	0	0	0
1	B	245	1833	1160	319	349	5	0	0	0
1	C	247	1867	1180	321	361	5	0	0	0
1	D	242	1794	1136	311	342	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

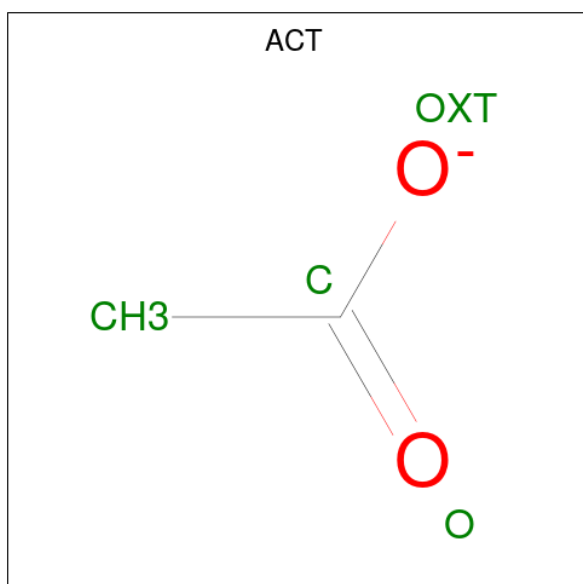
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P07669
B	?	-	GLU	deletion	UNP P07669
C	?	-	GLU	deletion	UNP P07669
D	?	-	GLU	deletion	UNP P07669

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



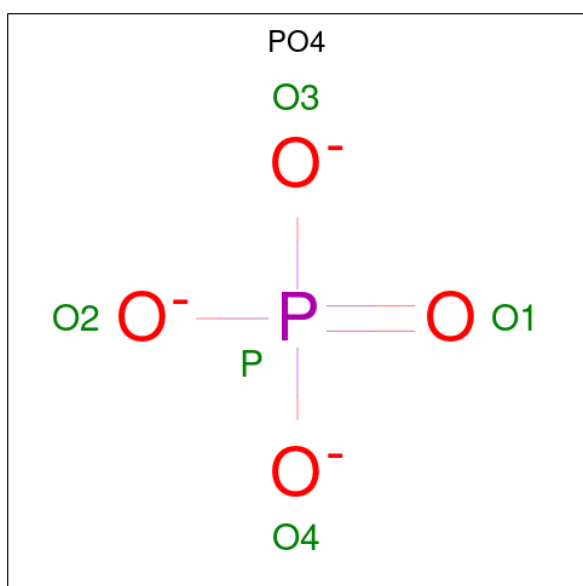
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O P 5 4 1	0	0

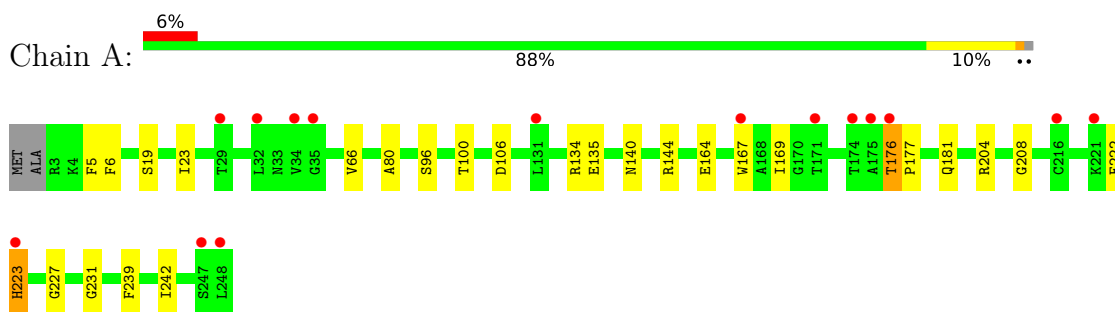
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	203	Total O 205 205	0	2
5	B	207	Total O 210 210	0	3
5	C	245	Total O 250 250	0	5
5	D	200	Total O 201 201	0	1

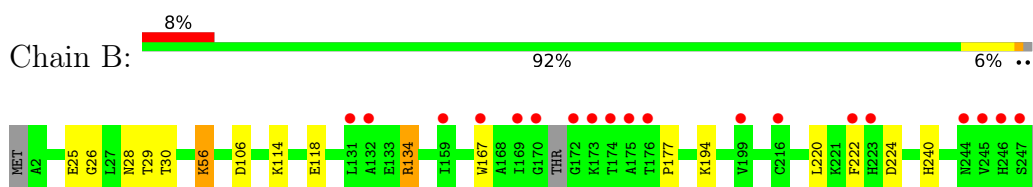
3 Residue-property plots [i](#)

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.

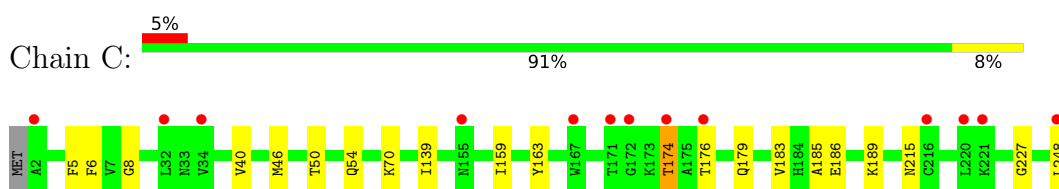
- Molecule 1: Triosephosphate isomerase



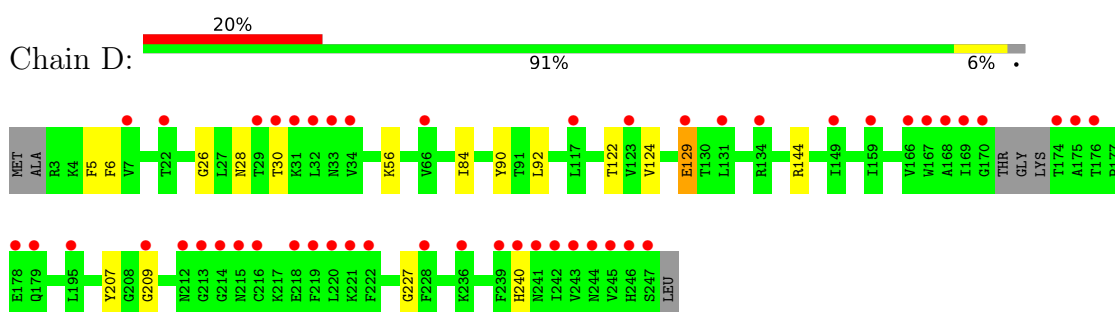
- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase



4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	149.51Å 149.51Å 99.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.38 – 1.79 47.28 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.38-1.79) 99.8 (47.28-1.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.79Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.218 0.181 , 0.217	Depositor DCC
R_{free} test set	2101 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8277	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: SO4, ACT, 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	0.69	0/1902	0.76	0/2577
1	B	0.72	0/1863	0.78	1/2525 (0.0%)
1	C	0.73	0/1897	0.81	0/2571
1	D	0.63	0/1823	0.73	0/2473
All	All	0.69	0/7485	0.77	1/10146 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ASP	CB-CG-OD1	5.00	122.80	118.30

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	1871	0	1836	17	0
1	B	1833	0	1777	11	0
1	C	1867	0	1824	16	0
1	D	1794	0	1712	11	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	8	0	6	1	0
3	C	8	0	6	1	0
4	C	5	0	0	0	0
5	A	205	0	0	2	0
5	B	210	0	0	3	0
5	C	250	0	0	2	0
5	D	201	0	0	3	0
All	All	8277	0	7161	56	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 4.

All (56) 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:176:THR:OG1	1:C:179:GLN:HG3	1.80	0.81
1:A:19:SER:O	1:A:23:ILE:HG13	1.88	0.73
1:B:28:ASN:HA	1:B:56:LYS:HD3	1.72	0.71
1:C:139:ILE:HD12	1:C:186:GLU:HG3	1.87	0.57
1:C:70:LYS:HD3	5:C:636:HOH:O	2.05	0.56
1:C:174:THR:HG21	1:C:215:ASN:ND2	2.21	0.55
1:A:140:ASN:ND2	1:A:140:ASN:H	2.06	0.54
1:A:140:ASN:H	1:A:140:ASN:HD22	1.55	0.54
1:B:224:ASP:HA	5:B:402:HOH:O	2.09	0.53
1:A:135:GLU:HB2	5:A:455:HOH:O	2.09	0.52
1:A:164:GLU:HG3	1:A:208:GLY:C	2.29	0.51
1:D:240:HIS:HE1	5:D:457:HOH:O	1.93	0.51
1:D:28:ASN:HA	1:D:56:LYS:HD3	1.93	0.51
1:A:231:GLY:N	3:A:302:ACT:H2	2.26	0.50
1:B:114:LYS:O	1:B:118:GLU:HG3	2.12	0.50
1:A:106:ASP:OD2	1:A:144:ARG:HD2	2.11	0.49
1:B:25:GLU:O	1:B:29:THR:HG23	2.13	0.49
1:C:174:THR:HG21	1:C:215:ASN:HD22	1.78	0.48
1:B:194:LYS:NZ	5:B:406:HOH:O	2.47	0.48
1:A:239:PHE:HA	1:A:242:ILE:HD12	1.95	0.47
1:A:134:ARG:HD3	1:A:167:TRP:CE2	2.49	0.47
1:D:5:PHE:CZ	1:D:227:GLY:HA2	2.50	0.47
1:A:66:VAL:HG21	1:A:80:ALA:HB2	1.97	0.47
1:A:176:THR:HG22	1:A:177:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:THR:HG21	1:B:240:HIS:CG	2.51	0.46
1:A:5:PHE:CZ	1:A:227:GLY:HA2	2.51	0.46
1:D:144:ARG:NH2	5:D:402:HOH:O	2.46	0.46
1:C:185:ALA:O	1:C:189:LYS:HG3	2.16	0.45
1:B:177:PRO:HB2	1:B:222:PHE:CE1	2.51	0.45
1:D:207:TYR:CZ	1:D:209:GLY:HA3	2.51	0.45
1:A:96:SER:O	1:A:100:THR:HG23	2.17	0.45
1:C:163:TYR:CZ	1:C:183:VAL:HG11	2.51	0.45
1:A:6:PHE:O	1:A:227:GLY:HA3	2.17	0.45
1:D:30:THR:HG21	1:D:240:HIS:CD2	2.53	0.44
1:D:26:GLY:O	1:D:30:THR:HG23	2.17	0.44
1:B:26:GLY:O	1:B:30:THR:HG23	2.17	0.44
1:C:46:MET:HG2	5:D:463:HOH:O	2.17	0.43
3:C:303:ACT:H3	5:C:631:HOH:O	2.18	0.43
1:C:159:ILE:HG23	1:C:159:ILE:HD12	1.62	0.43
1:B:25:GLU:HG3	5:B:579:HOH:O	2.18	0.43
1:D:129:GLU:H	1:D:129:GLU:HG3	1.56	0.43
1:C:70:LYS:HB2	1:C:70:LYS:NZ	2.33	0.43
1:B:134:ARG:HD3	1:B:167:TRP:CD2	2.54	0.42
1:D:6:PHE:O	1:D:227:GLY:HA3	2.19	0.42
1:A:164:GLU:OE2	1:A:169:ILE:HG12	2.20	0.41
1:C:6:PHE:O	1:C:227:GLY:HA3	2.20	0.41
1:C:50:THR:O	1:C:54:GLN:HG3	2.20	0.41
1:C:5:PHE:CZ	1:C:227:GLY:HA2	2.56	0.41
1:D:92:LEU:HD23	1:D:124:VAL:HB	2.02	0.41
1:C:139:ILE:CD1	1:C:186:GLU:HG3	2.51	0.41
1:C:248:LEU:HA	1:C:248:LEU:HD23	1.85	0.41
1:A:181:GLN:HG2	1:A:222:PHE:HD2	1.85	0.41
1:A:223:HIS:ND1	5:A:403:HOH:O	2.37	0.41
1:C:8:GLY:HA2	1:C:40:VAL:O	2.21	0.40
1:D:90:TYR:CD2	1:D:122:THR:HB	2.56	0.40
1:B:25:GLU:OE2	1:B:25:GLU:HA	2.21	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	244/248 (98%)	238 (98%)	6 (2%)	0	100	100
1	B	241/248 (97%)	235 (98%)	6 (2%)	0	100	100
1	C	245/248 (99%)	240 (98%)	5 (2%)	0	100	100
1	D	238/248 (96%)	232 (98%)	6 (2%)	0	100	100
All	All	968/992 (98%)	945 (98%)	23 (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	195/203 (96%)	192 (98%)	3 (2%)	65	56
1	B	185/203 (91%)	182 (98%)	3 (2%)	62	54
1	C	192/203 (95%)	191 (100%)	1 (0%)	88	87
1	D	176/203 (87%)	174 (99%)	2 (1%)	73	68
All	All	748/812 (92%)	739 (99%)	9 (1%)	71	65

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

Mol	Chain	Res	Type
1	A	176	THR
1	A	204	ARG
1	A	223	HIS
1	B	56	LYS
1	B	134	ARG
1	B	220	LEU
1	C	174	THR
1	D	84	ILE

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Mol	Chain	Res	Type
1	D	129	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	B	137	ASN
1	B	193	ASN
1	B	244	ASN

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](#)

10 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	$\# Z > 2$
4	PO4	C	304	-	4,4,4	0.95	0	6,6,6	1.31	1 (16%)
2	SO4	A	301	-	4,4,4	0.17	0	6,6,6	0.55	0
3	ACT	A	303	-	3,3,3	1.33	0	3,3,3	1.59	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	302	-	4,4,4	0.30	0	6,6,6	0.48	0
3	ACT	C	301	-	3,3,3	2.06	2 (66%)	3,3,3	1.10	0
3	ACT	C	303	-	3,3,3	1.22	0	3,3,3	1.34	0
2	SO4	C	302	-	4,4,4	0.49	0	6,6,6	0.31	0
2	SO4	D	301	-	4,4,4	0.47	0	6,6,6	0.53	0
3	ACT	A	302	-	3,3,3	1.86	1 (33%)	3,3,3	1.16	0
2	SO4	B	301	-	4,4,4	0.26	0	6,6,6	0.42	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	ACT	CH3-C	2.83	1.61	1.49
3	C	301	ACT	CH3-C	2.75	1.60	1.49
3	C	301	ACT	OXT-C	-2.26	1.19	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	304	PO4	O2-P-O1	2.28	119.24	110.89
3	A	303	ACT	O-C-CH3	-2.03	114.43	122.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	303	ACT	1	0
3	A	302	ACT	1	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

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, 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	246/248 (99%)	0.40	15 (6%) 21 16	27, 39, 57, 75	0
1	B	245/248 (98%)	0.55	19 (7%) 13 10	27, 37, 58, 88	0
1	C	247/248 (99%)	0.40	13 (5%) 26 21	26, 34, 50, 74	0
1	D	242/248 (97%)	1.18	49 (20%) 1 0	25, 40, 69, 88	0
All	All	980/992 (98%)	0.63	96 (9%) 7 5	25, 37, 60, 88	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	216	CYS	7.8
1	D	168	ALA	7.5
1	D	167	TRP	6.3
1	B	174	THR	6.3
1	D	222	PHE	6.2
1	D	176	THR	6.1
1	D	214	GLY	5.9
1	D	213	GLY	5.8
1	D	29	THR	5.6
1	A	223	HIS	5.5
1	D	175	ALA	5.2
1	D	220	LEU	5.1
1	D	246	HIS	4.9
1	D	219	PHE	4.8
1	D	174	THR	4.8
1	A	32	LEU	4.7
1	A	176	THR	4.5
1	B	223	HIS	4.4
1	D	245	VAL	4.4
1	D	169	ILE	4.4
1	D	34	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	248	LEU	4.3
1	B	173	LYS	4.1
1	D	30	THR	4.1
1	D	131	LEU	4.0
1	D	242	ILE	4.0
1	C	2	ALA	3.9
1	D	247	SER	3.9
1	D	243	VAL	3.9
1	D	166	VAL	3.6
1	D	31	LYS	3.6
1	D	228	PHE	3.5
1	B	131	LEU	3.5
1	B	172	GLY	3.5
1	D	32	LEU	3.5
1	C	171	THR	3.4
1	D	244	ASN	3.3
1	B	170	GLY	3.3
1	A	29	THR	3.3
1	C	172	GLY	3.2
1	C	174	THR	3.2
1	C	34	VAL	3.2
1	A	167	TRP	3.2
1	D	159	ILE	3.1
1	B	245	VAL	3.1
1	D	170	GLY	3.1
1	C	167	TRP	3.1
1	A	171	THR	3.0
1	C	221	LYS	3.0
1	D	212	ASN	2.9
1	D	218	GLU	2.9
1	B	222	PHE	2.9
1	D	239	PHE	2.9
1	D	236	LYS	2.9
1	D	240	HIS	2.9
1	B	216	CYS	2.8
1	A	175	ALA	2.8
1	C	220	LEU	2.8
1	B	175	ALA	2.8
1	B	132	ALA	2.7
1	B	176	THR	2.7
1	A	247	SER	2.6
1	D	33	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	221	LYS	2.6
1	A	216	CYS	2.6
1	B	169	ILE	2.6
1	C	32	LEU	2.6
1	C	216	CYS	2.6
1	D	134	ARG	2.5
1	D	241	ASN	2.5
1	B	246	HIS	2.4
1	A	34	VAL	2.4
1	D	123	VAL	2.4
1	B	167	TRP	2.4
1	B	199	VAL	2.4
1	D	215	ASN	2.4
1	D	179	GLN	2.4
1	B	244	ASN	2.4
1	C	155	ASN	2.3
1	A	35	GLY	2.3
1	A	174	THR	2.3
1	B	247	SER	2.3
1	D	66	VAL	2.3
1	A	248	LEU	2.3
1	D	209	GLY	2.2
1	A	131	LEU	2.2
1	A	221	LYS	2.2
1	D	22	THR	2.1
1	D	149	ILE	2.1
1	D	7	VAL	2.1
1	D	117	LEU	2.1
1	D	195	LEU	2.1
1	B	159	ILE	2.1
1	D	129	GLU	2.1
1	C	176	THR	2.0
1	D	178	GLU	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](#)

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	SO4	B	301	5/5	0.74	0.25	70,73,88,96	0
2	SO4	B	302	5/5	0.80	0.19	76,79,82,107	0
3	ACT	A	303	4/4	0.86	0.15	40,45,46,48	0
4	PO4	C	304	5/5	0.89	0.21	41,44,46,46	0
2	SO4	D	301	5/5	0.93	0.17	52,53,64,65	0
3	ACT	C	303	4/4	0.94	0.25	49,54,57,67	0
3	ACT	A	302	4/4	0.97	0.13	35,37,37,38	0
3	ACT	C	301	4/4	0.98	0.12	29,32,34,35	0
2	SO4	C	302	5/5	0.98	0.09	35,36,40,41	0
2	SO4	A	301	5/5	0.98	0.16	40,40,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.