



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:52 AM UTC

PDB ID : 3QTG / pdb_00003qtg
Title : Crystal structure of pyruvate kinase from *Pyrobaculum aerophilum*
Authors : Davies, C.; Solomons, J.T.G.
Deposited on : 2011-02-22
Resolution : 2.20 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

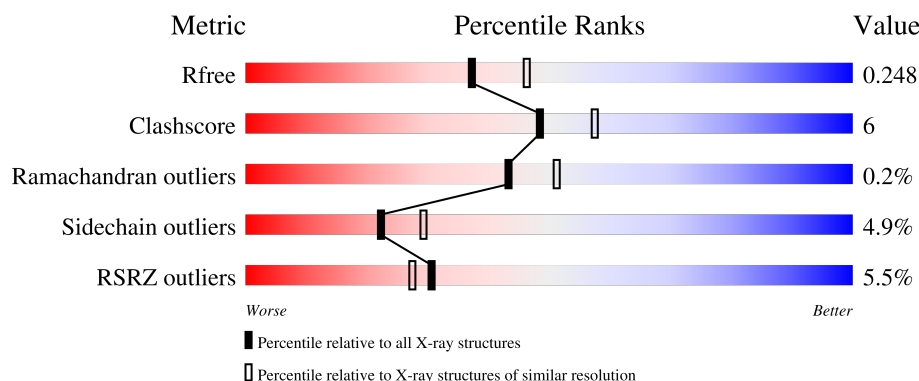
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	461	2% 82% 14% • •
1	B	461	8% 78% 12% • 9%

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
2	SO4	B	500	-	-	X	-
2	SO4	B	501	-	-	X	-

2 Entry composition [i](#)

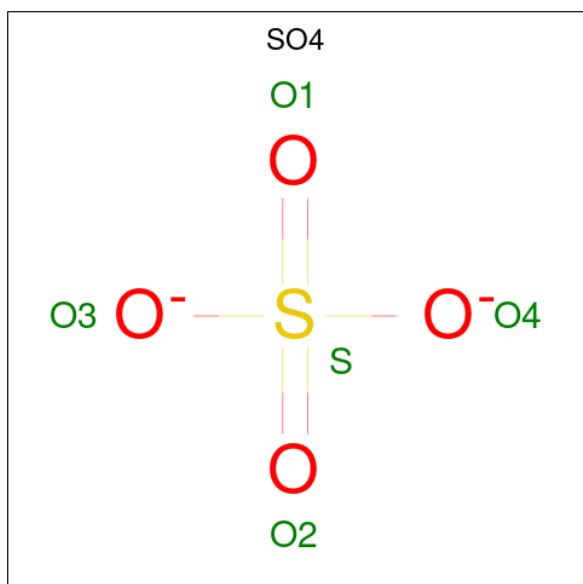
There are 3 unique types of molecules in this entry. The entry contains 6889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	2	0
			3473	2204	602	660	7			
1	B	419	Total	C	N	O	S	0	3	0
			3261	2077	566	611	7			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

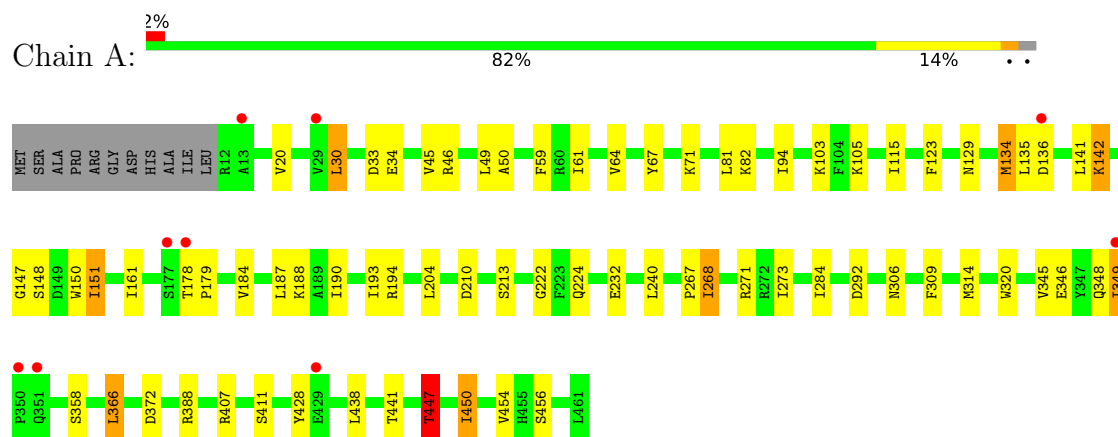
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total 70	O 70	0	0
3	B	70	Total 70	O 70	0	0

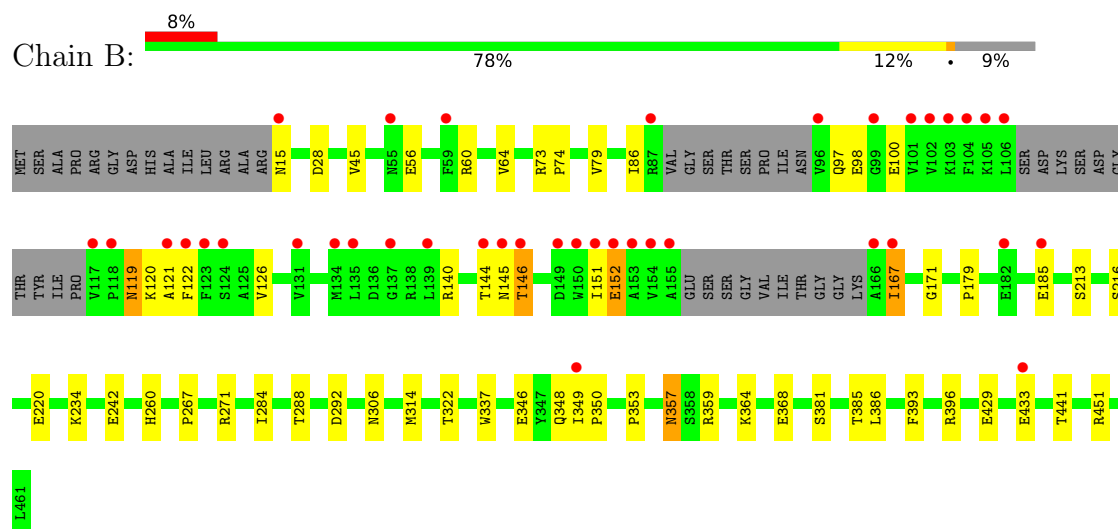
3 Residue-property plots [i](#)

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: Pyruvate kinase



• Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.30Å 107.40Å 105.00Å 90.00° 110.50° 90.00°	Depositor
Resolution (Å)	39.00 – 2.20 39.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.00-2.20) 99.4 (39.00-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.247 0.204 , 0.248	Depositor DCC
R_{free} test set	3110 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6889	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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

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	0.74	0/3534	0.93	1/4798 (0.0%)
1	B	0.76	2/3320 (0.1%)	0.92	3/4503 (0.1%)
All	All	0.75	2/6854 (0.0%)	0.93	4/9301 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	THR	CB-OG1	-7.87	1.31	1.43
1	B	144	THR	CB-OG1	-5.24	1.35	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	THR	OG1-CB-CG2	5.33	119.97	109.30
1	A	447	THR	N-CA-C	5.33	117.29	109.24
1	B	292	ASP	N-CA-C	5.33	117.50	111.11
1	B	337	TRP	N-CA-C	5.24	117.07	111.36

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	3473	0	3579	41	0
1	B	3261	0	3370	36	0
2	A	5	0	0	0	0
2	B	10	0	0	8	0
3	A	70	0	0	1	0
3	B	70	0	0	3	0
All	All	6889	0	6949	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 6.

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:A:103:LYS:HE2	1:A:105:LYS:HE2	1.46	0.94
2:B:501:SO4:O4	3:B:518:HOH:O	1.88	0.92
2:B:500:SO4:O3	3:B:517:HOH:O	1.92	0.86
1:B:97:GLN:HG3	1:B:100:GLU:HB2	1.56	0.84
1:A:50:ALA:HB2	1:A:82:LYS:HD3	1.60	0.84
1:B:350:PRO:HD3	1:B:396[B]:ARG:NH2	1.99	0.78
1:B:56:GLU:O	1:B:60:ARG:HG3	1.84	0.77
1:B:381:SER:OG	2:B:500:SO4:O2	2.00	0.77
2:B:500:SO4:O4	3:B:467:HOH:O	2.05	0.74
1:A:94:ILE:HD13	1:A:115:ILE:CD1	2.20	0.71
1:A:94:ILE:HD13	1:A:115:ILE:HD13	1.73	0.71
1:B:350:PRO:HD3	1:B:396[B]:ARG:HH21	1.59	0.66
1:A:271:ARG:HA	1:A:314:MET:HE1	1.82	0.62
1:A:123:PHE:CD1	1:A:151:ILE:HD12	2.34	0.61
1:A:447:THR:HG22	1:A:456:SER:O	2.01	0.60
1:B:359:ARG:HD3	2:B:501:SO4:O2	2.04	0.58
1:B:179:PRO:HD3	1:B:213:SER:HB3	1.85	0.58
1:B:288:THR:HG22	1:B:322:THR:HG21	1.86	0.57
1:A:366:LEU:HD21	1:A:447:THR:HG21	1.85	0.57
1:A:346:GLU:HG3	1:B:271:ARG:NH2	2.21	0.56
1:A:50:ALA:CB	1:A:82:LYS:HD3	2.33	0.55
1:A:306:ASN:ND2	1:B:267:PRO:HG3	2.22	0.55
1:B:28:ASP:OD1	1:B:60:ARG:HD3	2.08	0.54
1:A:178:THR:HB	1:A:179:PRO:HA	1.90	0.52
1:A:267:PRO:HG3	1:B:306:ASN:ND2	2.24	0.52
1:A:49:LEU:HD12	1:A:81:LEU:HD23	1.92	0.52
1:A:184:VAL:O	1:A:188:LYS:HG2	2.10	0.52
1:B:171:GLY:H	1:B:260:HIS:HD2	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HD21	1:A:273:ILE:HA	1.93	0.50
1:B:86:ILE:HG22	1:B:167:ILE:HG12	1.94	0.50
1:B:451:ARG:HA	2:B:501:SO4:O2	2.11	0.50
1:B:271:ARG:HA	1:B:314:MET:HE1	1.94	0.50
1:A:30:LEU:HG	1:A:34[B]:GLU:HB3	1.93	0.50
1:B:119:ASN:HD22	1:B:121:ALA:H	1.60	0.49
1:A:179:PRO:HD3	1:A:213:SER:HB3	1.94	0.49
1:A:268:ILE:HD11	1:B:346:GLU:HB2	1.95	0.48
1:A:366:LEU:HD21	1:A:447:THR:CG2	2.44	0.48
1:A:103:LYS:CE	1:A:105:LYS:HE2	2.32	0.48
1:B:216:SER:O	1:B:220:GLU:HG3	2.14	0.48
1:A:204:LEU:N	1:A:232:GLU:OE2	2.38	0.48
1:A:147:GLY:HA3	1:A:150:TRP:CE2	2.49	0.47
1:B:120:LYS:HE3	1:B:120:LYS:HB2	1.74	0.47
1:A:45:VAL:HG21	1:A:64:VAL:HG21	1.97	0.46
1:B:429:GLU:O	1:B:433:GLU:HG3	2.15	0.46
1:A:46:ARG:NH2	3:A:506:HOH:O	2.46	0.46
1:B:122:PHE:O	1:B:126:VAL:HG23	2.16	0.46
1:B:73:ARG:HA	1:B:74:PRO:HD3	1.70	0.46
1:A:348:GLN:O	1:A:349:ILE:C	2.59	0.46
1:A:428:TYR:OH	1:A:450:ILE:HG23	2.16	0.46
1:A:268:ILE:HA	1:A:268:ILE:HD13	1.68	0.45
1:B:86:ILE:HD13	1:B:122:PHE:HB2	1.98	0.45
1:B:364:LYS:O	1:B:368:GLU:HG3	2.17	0.45
1:B:45:VAL:HG21	1:B:64:VAL:HG21	1.99	0.45
1:B:353:PRO:HG2	1:B:393:PHE:CE1	2.52	0.45
1:B:385:THR:HB	2:B:500:SO4:O1	2.17	0.45
1:A:20:VAL:HB	1:A:320:TRP:CD1	2.52	0.44
1:A:224:GLN:HB2	1:A:407:ARG:NH2	2.32	0.44
1:B:171:GLY:HA2	1:B:234:LYS:HD2	1.99	0.44
1:B:145:ASN:HB2	1:B:152:GLU:HG2	1.99	0.44
1:A:388:ARG:NH2	1:A:411:SER:OG	2.51	0.43
1:A:61:ILE:HD12	1:A:193:ILE:HD12	2.00	0.43
1:A:123:PHE:HD1	1:A:151:ILE:HD12	1.79	0.42
1:A:309:PHE:CE1	1:A:345:VAL:HA	2.54	0.42
1:B:28:ASP:OD2	1:B:60:ARG:NH1	2.51	0.42
1:B:350:PRO:CD	1:B:396[B]:ARG:HH21	2.30	0.42
1:A:67:TYR:CE1	1:A:71:LYS:HG3	2.55	0.42
1:A:94:ILE:HD13	1:A:115:ILE:HD12	2.00	0.42
1:A:134:MET:HE1	1:A:161:ILE:HD13	2.02	0.41
1:A:178:THR:OG1	1:A:210:ASP:OD1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:LEU:N	2:B:500:SO4:O1	2.53	0.41
1:A:129:ASN:O	1:A:142:LYS:HE2	2.20	0.41
1:A:428:TYR:OH	1:A:450:ILE:CG2	2.69	0.41
1:A:194:ARG:HD2	1:A:222:GLY:C	2.46	0.41
1:B:357:ASN:HD22	1:B:359:ARG:H	1.68	0.41

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	450/461 (98%)	435 (97%)	13 (3%)	2 (0%)	30	34
1	B	414/461 (90%)	402 (97%)	12 (3%)	0	100	100
All	All	864/922 (94%)	837 (97%)	25 (3%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	SER
1	A	349	ILE

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	385/391 (98%)	363 (94%)	22 (6%)	18	23
1	B	361/391 (92%)	347 (96%)	14 (4%)	28	39
All	All	746/782 (95%)	710 (95%)	36 (5%)	22	30

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	33	ASP
1	A	59	PHE
1	A	134	MET
1	A	135	LEU
1	A	136	ASP
1	A	141	LEU
1	A	142	LYS
1	A	151	ILE
1	A	187	LEU
1	A	190	ILE
1	A	268	ILE
1	A	284	ILE
1	A	292	ASP
1	A	358	SER
1	A	366	LEU
1	A	372	ASP
1	A	438	LEU
1	A	441	THR
1	A	447	THR
1	A	450	ILE
1	A	454	VAL
1	B	15	ASN
1	B	79	VAL
1	B	98	GLU
1	B	119	ASN
1	B	140	ARG
1	B	146	THR
1	B	151	ILE
1	B	152	GLU
1	B	167	ILE
1	B	185	GLU
1	B	242	GLU
1	B	284	ILE
1	B	357	ASN

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Mol	Chain	Res	Type
1	B	441	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	97	GLN
1	A	306	ASN
1	B	15	ASN
1	B	55	ASN
1	B	119	ASN
1	B	129	ASN
1	B	260	HIS
1	B	306	ASN
1	B	357	ASN
1	B	371	GLN

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](#)

3 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	SO4	B	501	-	4,4,4	0.24	0	6,6,6	0.54	0
2	SO4	A	500	-	4,4,4	0.24	0	6,6,6	0.27	0
2	SO4	B	500	-	4,4,4	0.32	0	6,6,6	0.40	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	SO4	3	0
2	B	500	SO4	5	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	450/461 (97%)	0.27	9 (2%) 65 62	23, 46, 62, 76	2 (0%)
1	B	419/461 (90%)	0.40	39 (9%) 14 12	16, 43, 93, 103	3 (0%)
All	All	869/922 (94%)	0.33	48 (5%) 30 27	16, 45, 83, 103	5 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	ALA	5.4
1	B	144	THR	4.6
1	B	154	VAL	4.6
1	B	106	LEU	4.5
1	B	101	VAL	4.2
1	B	96	VAL	4.1
1	B	104	PHE	4.1
1	B	102	VAL	4.1
1	B	15	ASN	4.0
1	B	146	THR	3.7
1	B	151	ILE	3.6
1	A	351	GLN	3.5
1	B	87	ARG	3.5
1	B	135	LEU	3.5
1	B	105	LYS	3.4
1	B	349	ILE	3.2
1	B	117	VAL	3.2
1	B	150	TRP	3.2
1	B	153	ALA	3.2
1	A	349	ILE	3.2
1	A	13	ALA	2.9
1	B	139	LEU	2.9
1	B	167	ILE	2.9
1	A	350	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	122	PHE	2.8
1	B	123	PHE	2.7
1	B	118	PRO	2.7
1	B	166	ALA	2.6
1	A	178	THR	2.5
1	B	121	ALA	2.5
1	B	149	ASP	2.5
1	B	99	GLY	2.5
1	B	131	VAL	2.5
1	B	59	PHE	2.4
1	B	124	SER	2.2
1	B	152	GLU	2.2
1	A	29	VAL	2.1
1	B	433	GLU	2.1
1	B	134	MET	2.1
1	B	55	ASN	2.1
1	B	182	GLU	2.1
1	B	137	GLY	2.1
1	A	136	ASP	2.1
1	A	177	SER	2.0
1	B	103	LYS	2.0
1	A	429	GLU	2.0
1	B	185	GLU	2.0
1	B	145	ASN	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 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($\text{\AA}^2$)	Q<0.9
2	SO4	B	501	5/5	0.93	0.17	44,45,48,48	5
2	SO4	B	500	5/5	0.97	0.13	21,29,31,31	5
2	SO4	A	500	5/5	0.98	0.05	39,41,42,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.