



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:45 pm BST

PDB ID : 6W8T
Title : Crystal structure of metacaspase 4 from Arabidopsis (microcrystals treated with calcium)
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Deposited on : 2020-03-21
Resolution : 3.20 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 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

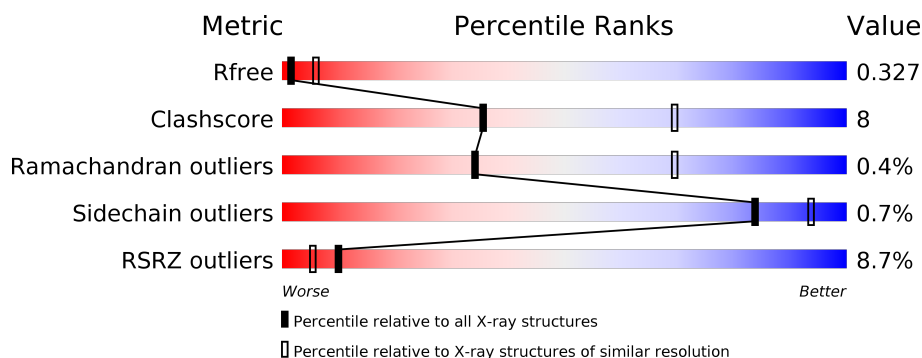
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	426	<div> <div>4%</div> <div>68%</div> <div>16%</div> <div>16%</div> </div>
1	B	426	<div> <div>10%</div> <div>64%</div> <div>15%</div> <div>21%</div> </div>

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	A	501	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5233 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 Metacaspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2704	1669	461	556	18			
1	B	335	Total	C	N	O	S	0	0	0
			2524	1561	432	513	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	VAL	-	expression tag	UNP O64517
A	420	GLU	-	expression tag	UNP O64517
A	421	HIS	-	expression tag	UNP O64517
A	422	HIS	-	expression tag	UNP O64517
A	423	HIS	-	expression tag	UNP O64517
A	424	HIS	-	expression tag	UNP O64517
A	425	HIS	-	expression tag	UNP O64517
A	426	HIS	-	expression tag	UNP O64517
B	419	VAL	-	expression tag	UNP O64517
B	420	GLU	-	expression tag	UNP O64517
B	421	HIS	-	expression tag	UNP O64517
B	422	HIS	-	expression tag	UNP O64517
B	423	HIS	-	expression tag	UNP O64517
B	424	HIS	-	expression tag	UNP O64517
B	425	HIS	-	expression tag	UNP O64517
B	426	HIS	-	expression tag	UNP O64517

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

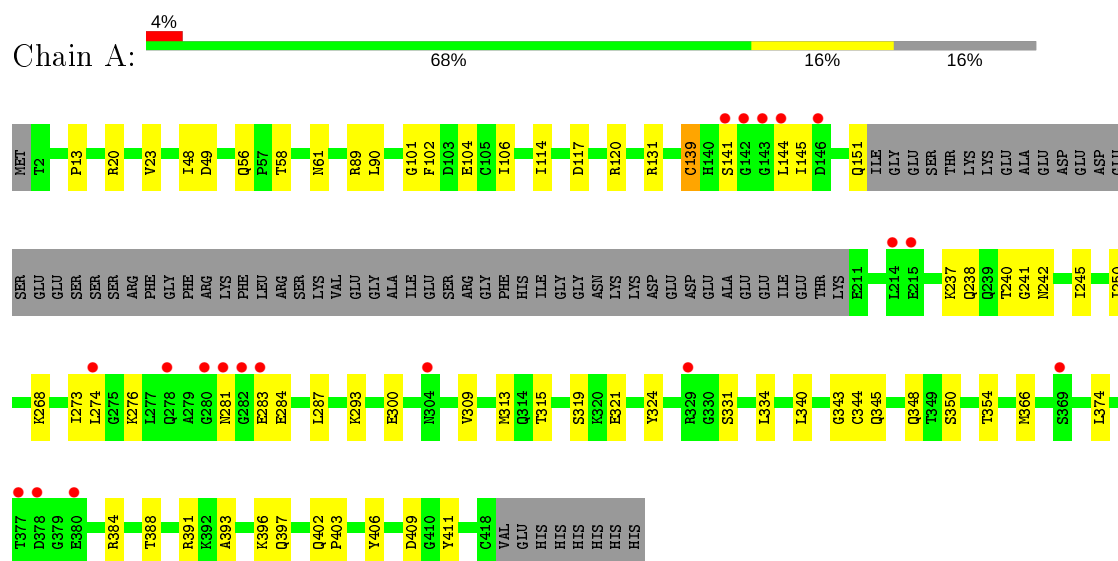


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

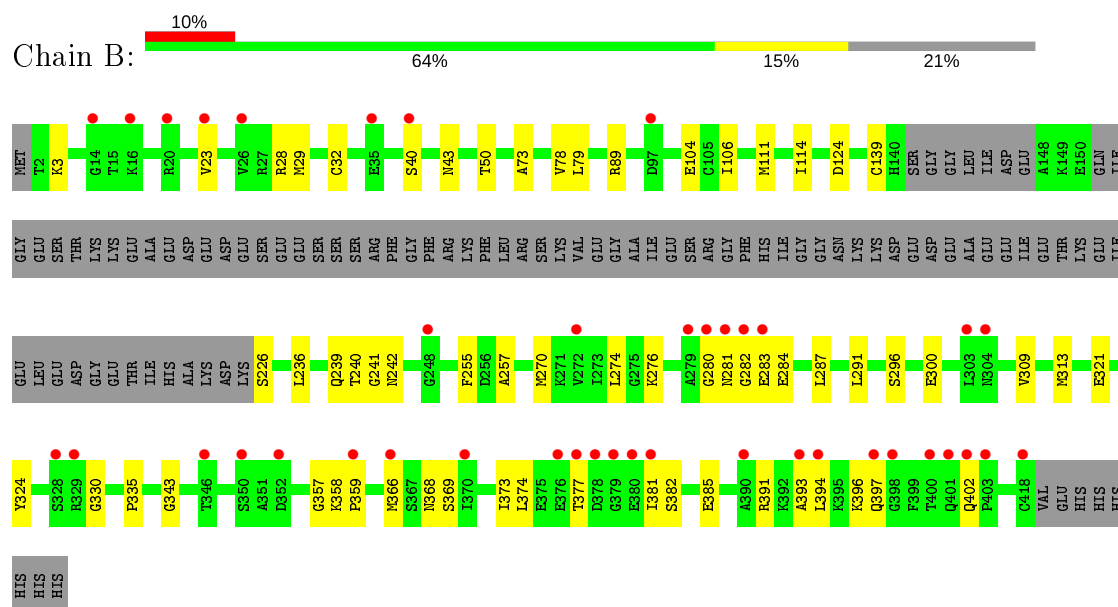
3 Residue-property plots [i](#)

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: Metacaspase-4



• Molecule 1: Metacaspase-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	49.34Å 58.06Å 300.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 3.20 38.15 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.8 (38.00-3.20) 91.9 (38.15-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.286 , 0.321 0.289 , 0.327	Depositor DCC
R_{free} test set	731 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	5233	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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

5.1 Standard geometry

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	0.26	0/2742	0.45	0/3698
1	B	0.26	0/2560	0.44	0/3453
All	All	0.26	0/5302	0.45	0/7151

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	2704	0	2652	48	0
1	B	2524	0	2481	39	0
2	A	5	0	0	4	0
All	All	5233	0	5133	84	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 8.

All (84) 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:276:LYS:HE3	1:B:283:GLU:HB3	1.63	0.79
1:A:345:GLN:H	1:A:348:GLN:HE21	1.34	0.76
1:A:293:LYS:HB2	2:A:501:SO4:O1	1.86	0.74
1:A:276:LYS:HE3	1:A:283:GLU:HB3	1.69	0.74
1:A:145:ILE:HG21	1:A:406:TYR:HB3	1.72	0.71
1:B:89:ARG:HD2	1:B:104:GLU:HG2	1.74	0.69
1:A:344:CYS:HB2	1:A:348:GLN:HG3	1.75	0.68
1:A:151:GLN:NE2	1:A:388:THR:OG1	2.27	0.67
1:A:120:ARG:HH21	1:A:331:SER:HB2	1.60	0.66
1:A:293:LYS:HD2	2:A:501:SO4:O4	1.97	0.64
1:A:238:GLN:OE1	1:B:357:GLY:HA3	1.98	0.62
1:A:117:ASP:OD1	1:A:120:ARG:NH2	2.32	0.62
1:A:120:ARG:HH11	1:A:144:LEU:HA	1.65	0.61
1:A:145:ILE:HG12	1:A:334:LEU:HD22	1.82	0.61
1:B:309:VAL:HG12	1:B:313:MET:HG2	1.80	0.61
1:B:106:ILE:HG12	1:B:114:ILE:HB	1.83	0.60
1:B:139:CYS:HG	1:B:226:SER:N	1.99	0.60
1:B:391:ARG:O	1:B:402:GLN:NE2	2.35	0.58
1:A:120:ARG:HD3	1:A:144:LEU:HA	1.85	0.58
1:A:120:ARG:NH1	1:A:144:LEU:HA	2.19	0.57
1:A:145:ILE:HD13	1:A:340:LEU:HD22	1.88	0.56
1:A:281:ASN:ND2	1:A:284:GLU:OE2	2.39	0.55
1:A:309:VAL:HG12	1:A:313:MET:HG2	1.88	0.55
1:B:240:THR:O	1:B:242:ASN:N	2.40	0.54
1:A:89:ARG:HD2	1:A:104:GLU:HG2	1.91	0.53
1:A:106:ILE:HG12	1:A:114:ILE:HB	1.92	0.52
1:A:345:GLN:H	1:A:348:GLN:NE2	2.04	0.52
1:A:343:GLY:HA2	1:A:366:MET:HG3	1.92	0.52
1:A:20:ARG:HH11	1:A:354:THR:HG21	1.75	0.50
1:A:240:THR:O	1:A:242:ASN:N	2.40	0.50
1:A:139:CYS:HB3	1:A:350:SER:H	1.76	0.50
1:A:58:THR:OG1	1:A:61:ASN:OD1	2.29	0.50
1:B:23:VAL:HG21	1:B:50:THR:HG23	1.93	0.50
1:B:73:ALA:HB2	1:B:79:LEU:HD11	1.94	0.49
1:B:29:MET:HA	1:B:32:CYS:HB3	1.93	0.49
1:B:393:ALA:O	1:B:396:LYS:HG2	2.12	0.49
1:A:348:GLN:NE2	1:A:402:GLN:H	2.10	0.49
1:B:240:THR:C	1:B:242:ASN:H	2.14	0.49
1:A:273:ILE:HB	1:A:287:LEU:HD11	1.95	0.49
1:A:391:ARG:NH1	1:A:403:PRO:O	2.44	0.49
1:B:28:ARG:HH22	1:B:368:ASN:HB2	1.77	0.49
1:A:13:PRO:O	1:B:359:PRO:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD11	1:A:250:ILE:HG21	1.95	0.48
1:B:111:MET:HG2	1:B:239:GLN:HG3	1.95	0.47
1:A:49:ASP:HA	1:A:56:GLN:HE22	1.79	0.47
1:B:3:LYS:HG2	1:B:78:VAL:HB	1.98	0.46
1:B:40:SER:OG	1:B:43:ASN:ND2	2.49	0.46
1:B:281:ASN:ND2	1:B:284:GLU:OE2	2.48	0.46
1:A:23:VAL:HG13	1:A:48:ILE:HD13	1.98	0.46
1:A:293:LYS:CD	2:A:501:SO4:O4	2.64	0.46
1:B:124:ASP:HA	1:B:335:PRO:HG2	1.98	0.45
1:A:237:LYS:HG2	1:A:245:ILE:HB	1.98	0.45
1:B:287:LEU:HD21	1:B:291:LEU:HD12	1.97	0.45
1:B:106:ILE:HD11	1:B:114:ILE:HD12	1.98	0.45
1:B:343:GLY:HA2	1:B:366:MET:HG3	1.99	0.45
1:B:240:THR:HG21	1:B:257:ALA:CB	2.47	0.44
1:A:396:LYS:HG3	1:A:397:GLN:HE21	1.81	0.44
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.83	0.44
1:B:255:PHE:CG	1:B:270:MET:HG3	2.53	0.44
1:A:321:GLU:HG3	1:A:324:TYR:CE2	2.53	0.44
1:B:274:LEU:HD13	1:B:309:VAL:HG13	1.99	0.44
1:B:377:THR:HG21	1:B:381:ILE:HD12	1.99	0.43
1:B:373:ILE:O	1:B:377:THR:HG23	2.19	0.43
1:A:274:LEU:HD13	1:A:309:VAL:HG13	2.00	0.43
1:B:396:LYS:HG3	1:B:397:GLN:HE21	1.83	0.43
1:A:238:GLN:O	1:B:358:LYS:HD3	2.19	0.43
1:A:319:SER:OG	1:A:321:GLU:OE1	2.35	0.43
1:B:369:SER:HB2	1:B:394:LEU:HD21	2.01	0.43
1:B:28:ARG:HE	1:B:28:ARG:HB2	1.70	0.43
1:B:374:LEU:HA	1:B:374:LEU:HD23	1.85	0.42
1:A:101:GLY:C	1:A:102:PHE:HD1	2.23	0.42
1:B:381:ILE:HA	1:B:385:GLU:OE1	2.18	0.42
1:A:348:GLN:HE22	1:A:402:GLN:HB2	1.85	0.42
1:B:382:SER:H	1:B:385:GLU:HB2	1.85	0.42
1:A:268:LYS:HG2	1:A:315:THR:HB	2.02	0.41
1:A:293:LYS:HB2	2:A:501:SO4:S	2.60	0.41
1:A:374:LEU:HA	1:A:374:LEU:HD23	1.77	0.41
1:A:131:ARG:HG2	1:A:411:TYR:CZ	2.56	0.41
1:B:296:SER:O	1:B:300:GLU:HB2	2.21	0.41
1:A:145:ILE:HG13	1:A:334:LEU:HB2	2.02	0.41
1:A:393:ALA:O	1:A:397:GLN:HG2	2.21	0.41
1:B:321:GLU:HG3	1:B:324:TYR:CE2	2.55	0.41
1:A:141:SER:O	1:A:144:LEU:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:GLY:O	1:B:282:GLY:N	2.54	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	354/426 (83%)	334 (94%)	19 (5%)	1 (0%)	41	74
1	B	329/426 (77%)	315 (96%)	12 (4%)	2 (1%)	25	64
All	All	683/852 (80%)	649 (95%)	31 (4%)	3 (0%)	34	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	241	GLY
1	A	241	GLY
1	B	330	GLY

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	298/357 (84%)	294 (99%)	4 (1%)	69	87
1	B	278/357 (78%)	278 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	576 / 714 (81%)	572 (99%)	4 (1%)	84	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	CYS
1	A	300	GLU
1	A	384	ARG
1	A	409	ASP

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

Mol	Chain	Res	Type
1	A	56	GLN
1	A	244	ASN
1	A	281	ASN
1	A	348	GLN
1	A	397	GLN
1	B	11	ASN
1	B	43	ASN
1	B	56	GLN
1	B	61	ASN
1	B	281	ASN
1	B	397	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	A	501	-	4,4,4	0.10	0	6,6,6	0.12	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.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	4	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	358/426 (84%)	0.28	19 (5%) 26 14	15, 56, 142, 213	0
1	B	335/426 (78%)	0.96	41 (12%) 4 2	27, 92, 147, 240	0
All	All	693/852 (81%)	0.61	60 (8%) 10 5	15, 73, 146, 240	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	ASN	10.5
1	A	282	GLY	7.3
1	B	378	ASP	7.3
1	B	377	THR	7.1
1	A	380	GLU	6.7
1	B	280	GLY	6.6
1	B	282	GLY	5.8
1	B	380	GLU	5.6
1	B	398	GLY	4.9
1	A	283	GLU	4.7
1	B	359	PRO	4.6
1	B	393	ALA	4.5
1	A	141	SER	4.4
1	B	328	SER	4.2
1	A	329	ARG	4.0
1	A	377	THR	4.0
1	A	143	GLY	3.9
1	A	378	ASP	3.8
1	B	379	GLY	3.8
1	B	400	THR	3.3
1	B	283	GLU	3.3
1	B	390	ALA	3.3
1	A	144	LEU	3.2
1	B	397	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	304	ASN	3.1
1	A	278	GLN	3.1
1	B	401	GLN	3.1
1	A	274	LEU	3.1
1	B	97	ASP	3.0
1	B	272	VAL	2.9
1	B	418	CYS	2.8
1	B	14	GLY	2.8
1	B	403	PRO	2.8
1	B	40	SER	2.7
1	B	303	LEU	2.7
1	B	26	VAL	2.7
1	A	280	GLY	2.7
1	B	366	MET	2.6
1	B	20	ARG	2.6
1	B	381	ILE	2.5
1	B	394	LEU	2.5
1	A	369	SER	2.5
1	B	350	SER	2.5
1	A	281	ASN	2.4
1	B	346	THR	2.4
1	B	35	GLU	2.4
1	B	279	ALA	2.4
1	B	16	LYS	2.3
1	A	142	GLY	2.3
1	A	146	ASP	2.3
1	B	304	ASN	2.2
1	B	329	ARG	2.2
1	B	370	ILE	2.2
1	B	248	GLY	2.1
1	B	23	VAL	2.1
1	B	402	GLN	2.1
1	A	214	LEU	2.1
1	A	215	GLU	2.0
1	B	376	GLU	2.0
1	B	352	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(\AA^2)	Q<0.9
2	SO4	A	501	5/5	0.92	0.16	98,100,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.