



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:04 PM UTC

PDB ID : 6W8R / pdb_00006w8r
Title : Crystal structure of metacaspase 4 C139A from Arabidopsis
Authors : Zhu, P.; Yu, X.H.; Wang, C.; Zhang, Q.; Liu, W.; McSweeney, S.; Shanklin, J.; Lam, E.; Liu, Q.
Deposited on : 2020-03-21
Resolution : 2.80 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

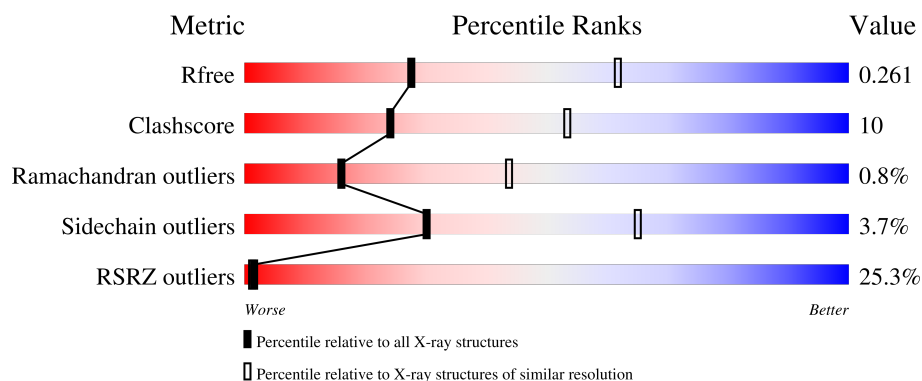
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	433	23% 63% 20% 16%
1	B	433	18% 61% 19% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5414 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	364	Total	C	N	O	S	0	0	0
			2741	1693	468	562	18			
1	B	352	Total	C	N	O	S	0	0	0
			2651	1639	454	541	17			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	ALA	CYS	engineered mutation	UNP O64517
A	419	VAL	-	expression tag	UNP O64517
A	420	ASP	-	expression tag	UNP O64517
A	421	LYS	-	expression tag	UNP O64517
A	422	LEU	-	expression tag	UNP O64517
A	423	ALA	-	expression tag	UNP O64517
A	424	ALA	-	expression tag	UNP O64517
A	425	ALA	-	expression tag	UNP O64517
A	426	LEU	-	expression tag	UNP O64517
A	427	GLU	-	expression tag	UNP O64517
A	428	HIS	-	expression tag	UNP O64517
A	429	HIS	-	expression tag	UNP O64517
A	430	HIS	-	expression tag	UNP O64517
A	431	HIS	-	expression tag	UNP O64517
A	432	HIS	-	expression tag	UNP O64517
A	433	HIS	-	expression tag	UNP O64517
B	139	ALA	CYS	engineered mutation	UNP O64517
B	419	VAL	-	expression tag	UNP O64517
B	420	ASP	-	expression tag	UNP O64517
B	421	LYS	-	expression tag	UNP O64517
B	422	LEU	-	expression tag	UNP O64517
B	423	ALA	-	expression tag	UNP O64517
B	424	ALA	-	expression tag	UNP O64517
B	425	ALA	-	expression tag	UNP O64517
B	426	LEU	-	expression tag	UNP O64517

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Chain	Residue	Modelled	Actual	Comment	Reference
B	427	GLU	-	expression tag	UNP O64517
B	428	HIS	-	expression tag	UNP O64517
B	429	HIS	-	expression tag	UNP O64517
B	430	HIS	-	expression tag	UNP O64517
B	431	HIS	-	expression tag	UNP O64517
B	432	HIS	-	expression tag	UNP O64517
B	433	HIS	-	expression tag	UNP O64517

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



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

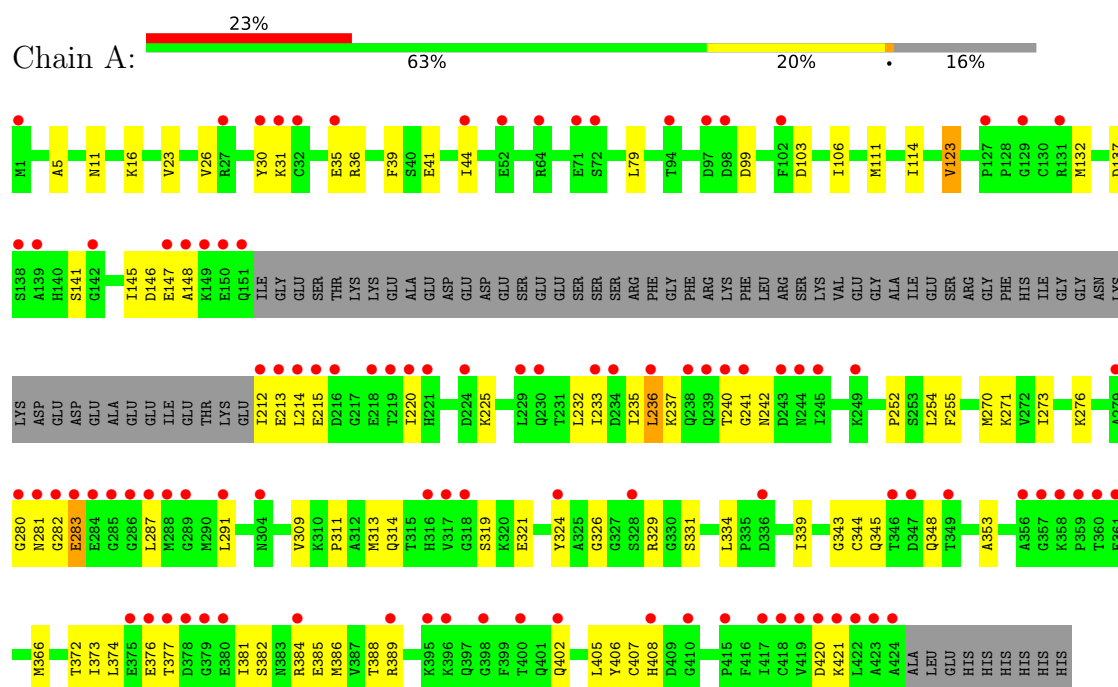
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	8	Total	O	0	0
			8	8		

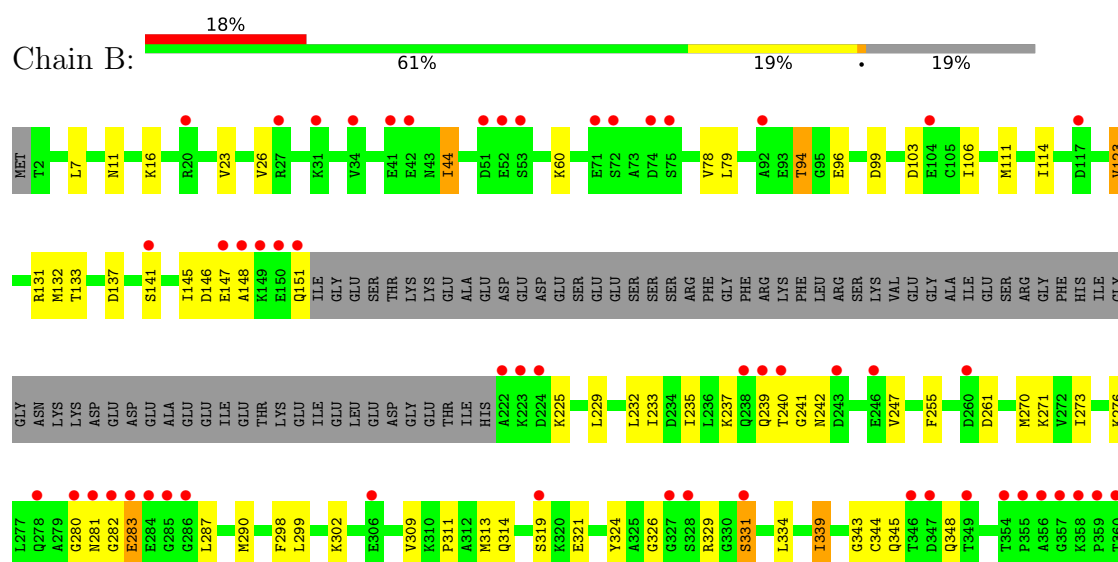
3 Residue-property plots [i](#)

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: Metacaspase-4



• Molecule 1: Metacaspase-4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.16Å 216.10Å 40.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.80 – 2.80 39.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.0 (39.80-2.80) 81.0 (39.80-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.248 , 0.266 0.244 , 0.261	Depositor DCC
R_{free} test set	981 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	5414	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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	0.18	0/2779	0.43	0/3748
1	B	0.17	0/2688	0.43	0/3625
All	All	0.18	0/5467	0.43	0/7373

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	2741	0	2696	55	0
1	B	2651	0	2616	55	0
2	B	5	0	0	1	0
3	A	9	0	0	0	0
3	B	8	0	0	0	0
All	All	5414	0	5312	107	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 10.

All (107) 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:151:GLN:HE22	1:B:405:LEU:HB3	1.35	0.91
1:A:339:ILE:HD11	1:A:405:LEU:HD11	1.64	0.80
1:A:31:LYS:HG2	1:B:419:VAL:HG11	1.69	0.73
1:B:131:ARG:NH2	1:B:415:PRO:O	2.22	0.72
1:B:133:THR:HG23	1:B:339:ILE:HD11	1.73	0.70
1:B:377:THR:HG21	1:B:389:ARG:NH1	2.07	0.69
1:A:276:LYS:HE3	1:A:283:GLU:HB3	1.76	0.68
1:B:94:THR:HG23	1:B:96:GLU:H	1.57	0.67
1:B:276:LYS:HE3	1:B:283:GLU:HB3	1.76	0.67
1:B:348:GLN:HE22	1:B:402:GLN:HB2	1.60	0.67
1:A:348:GLN:HE22	1:A:402:GLN:HB2	1.60	0.66
1:B:409:ASP:N	2:B:501:SO4:O3	2.30	0.64
1:A:146:ASP:HB2	1:A:331:SER:HA	1.80	0.64
1:A:345:GLN:H	1:A:348:GLN:NE2	1.97	0.62
1:B:111:MET:HE3	1:B:232:LEU:HD12	1.81	0.62
1:B:146:ASP:HB2	1:B:331:SER:HA	1.80	0.62
1:B:273:ILE:HB	1:B:287:LEU:HD11	1.81	0.62
1:A:344:CYS:HB2	1:A:348:GLN:HG3	1.82	0.61
1:A:111:MET:HE3	1:A:232:LEU:HD12	1.81	0.61
1:B:344:CYS:HB2	1:B:348:GLN:HG3	1.83	0.61
1:B:345:GLN:H	1:B:348:GLN:NE2	1.97	0.61
1:B:309:VAL:HG12	1:B:313:MET:HG2	1.83	0.60
1:A:273:ILE:HB	1:A:287:LEU:HD11	1.82	0.60
1:A:309:VAL:HG12	1:A:313:MET:HG2	1.83	0.59
1:A:343:GLY:HA2	1:A:366:MET:HG3	1.85	0.58
1:B:319:SER:OG	1:B:321:GLU:OE1	2.21	0.58
1:A:334:LEU:O	1:A:408:HIS:NE2	2.34	0.56
1:B:103:ASP:OD1	1:B:326:GLY:N	2.38	0.56
1:B:123:VAL:HG13	1:B:132:MET:HE1	1.87	0.56
1:B:106:ILE:HD11	1:B:114:ILE:HD12	1.88	0.56
1:B:345:GLN:H	1:B:348:GLN:HE21	1.54	0.56
1:A:123:VAL:HG13	1:A:132:MET:HE1	1.87	0.56
1:A:146:ASP:O	1:A:148:ALA:N	2.36	0.55
1:A:106:ILE:HD11	1:A:114:ILE:HD12	1.89	0.55
1:A:345:GLN:H	1:A:348:GLN:HE21	1.54	0.54
1:B:343:GLY:HA2	1:B:366:MET:HG3	1.88	0.54
1:A:31:LYS:HG2	1:B:419:VAL:CG1	2.38	0.53
1:B:229:LEU:HD23	1:B:247:VAL:HG22	1.91	0.53
1:B:334:LEU:O	1:B:408:HIS:NE2	2.35	0.53
1:B:151:GLN:HE22	1:B:405:LEU:CB	2.14	0.53
1:A:319:SER:OG	1:A:321:GLU:OE1	2.21	0.52
1:B:146:ASP:O	1:B:148:ALA:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:MET:HE2	1:A:235:ILE:HB	1.92	0.51
1:B:11:ASN:HD21	1:B:23:VAL:H	1.59	0.50
1:A:213:GLU:C	1:A:214:LEU:HD12	2.37	0.50
1:B:348:GLN:NE2	1:B:402:GLN:H	2.10	0.50
1:B:382:SER:OG	1:B:385:GLU:HG3	2.11	0.50
1:A:348:GLN:NE2	1:A:402:GLN:H	2.09	0.50
1:B:280:GLY:O	1:B:282:GLY:N	2.45	0.50
1:B:7:LEU:HD11	1:B:44:ILE:HD11	1.94	0.49
1:A:382:SER:OG	1:A:385:GLU:HG3	2.12	0.49
1:B:298:PHE:CZ	1:B:302:LYS:HE3	2.48	0.48
1:A:255:PHE:CG	1:A:270:MET:HG3	2.48	0.48
1:B:255:PHE:CG	1:B:270:MET:HG3	2.48	0.48
1:B:111:MET:HE2	1:B:235:ILE:HB	1.96	0.48
1:B:137:ASP:O	1:B:225:LYS:HE2	2.15	0.47
1:A:30:TYR:OH	1:A:41:GLU:HB3	2.15	0.47
1:A:79:LEU:O	1:A:132:MET:HA	2.15	0.46
1:B:79:LEU:O	1:B:132:MET:HA	2.16	0.46
1:A:420:ASP:CG	1:A:421:LYS:N	2.74	0.46
1:A:35:GLU:OE1	1:B:131:ARG:NH1	2.49	0.46
1:A:280:GLY:O	1:A:282:GLY:N	2.46	0.45
1:A:372:THR:O	1:A:376:GLU:HG2	2.16	0.45
1:A:145:ILE:HD13	1:A:406:TYR:CE1	2.52	0.45
1:A:11:ASN:HD21	1:A:23:VAL:H	1.63	0.45
1:A:384:ARG:O	1:A:388:THR:OG1	2.29	0.45
1:B:387:VAL:HG21	1:B:405:LEU:HB2	1.98	0.45
1:B:311:PRO:HA	1:B:314:GLN:NE2	2.31	0.44
1:B:372:THR:O	1:B:376:GLU:HG2	2.18	0.44
1:B:78:VAL:HG11	1:B:418:CYS:HB2	1.99	0.44
1:A:255:PHE:CZ	1:A:311:PRO:HG2	2.52	0.44
1:B:380:GLU:HG3	1:B:381:ILE:N	2.32	0.43
1:A:103:ASP:OD1	1:A:326:GLY:N	2.48	0.43
1:B:373:ILE:HD13	1:B:389:ARG:HB2	2.00	0.43
1:B:377:THR:HG21	1:B:389:ARG:HH11	1.78	0.43
1:A:5:ALA:HB3	1:A:44:ILE:HG23	2.00	0.43
1:A:233:ILE:O	1:A:237:LYS:HG3	2.19	0.43
1:A:271:LYS:CD	1:A:313:MET:HA	2.49	0.43
1:A:311:PRO:HA	1:A:314:GLN:NE2	2.34	0.43
1:B:145:ILE:HD13	1:B:406:TYR:CE1	2.54	0.43
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.81	0.43
1:B:240:THR:O	1:B:242:ASN:N	2.52	0.43
1:A:420:ASP:CG	1:A:421:LYS:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ILE:O	1:B:237:LYS:HG3	2.19	0.42
1:B:255:PHE:CZ	1:B:311:PRO:HG2	2.54	0.42
1:A:137:ASP:O	1:A:225:LYS:HE2	2.19	0.42
1:B:99:ASP:HB2	1:B:324:TYR:CD1	2.54	0.42
1:A:106:ILE:HG12	1:A:114:ILE:HB	2.01	0.42
1:B:271:LYS:CD	1:B:313:MET:HA	2.49	0.42
1:A:212:ILE:HG12	1:A:214:LEU:HD11	2.02	0.42
1:A:339:ILE:HG13	1:A:407:CYS:HB3	2.01	0.42
1:A:240:THR:O	1:A:242:ASN:N	2.53	0.41
1:A:146:ASP:C	1:A:148:ALA:H	2.25	0.41
1:A:373:ILE:HD13	1:A:389:ARG:HB2	2.02	0.41
1:A:236:LEU:HD11	1:A:254:LEU:HD21	2.03	0.41
1:A:276:LYS:HE2	1:A:287:LEU:HD12	2.02	0.41
1:A:374:LEU:HG	1:A:386:MET:HE1	2.01	0.41
1:B:60:LYS:HD2	1:B:261:ASP:OD2	2.20	0.41
1:A:39:PHE:HB3	1:A:44:ILE:HD11	2.02	0.41
1:A:252:PRO:HG2	1:A:291:LEU:HD21	2.03	0.41
1:B:106:ILE:HG12	1:B:114:ILE:HB	2.01	0.41
1:B:123:VAL:HG13	1:B:132:MET:CE	2.51	0.41
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.95	0.41
1:B:7:LEU:CD1	1:B:44:ILE:HD11	2.51	0.40
1:A:36:ARG:NH1	1:A:377:THR:O	2.55	0.40
1:A:99:ASP:HB2	1:A:324:TYR:CD1	2.56	0.40
1:A:220:ILE:HG21	1:A:353:ALA:HB1	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	360/433 (83%)	336 (93%)	21 (6%)	3 (1%)	16 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	348/433 (80%)	330 (95%)	15 (4%)	3 (1%)	14	41
All	All	708/866 (82%)	666 (94%)	36 (5%)	6 (1%)	16	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	GLY
1	B	241	GLY
1	A	147	GLU
1	B	147	GLU
1	B	281	ASN
1	A	281	ASN

5.3.2 Protein sidechains ⓘ

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	300/360 (83%)	291 (97%)	9 (3%)	36	72
1	B	291/360 (81%)	278 (96%)	13 (4%)	24	58
All	All	591/720 (82%)	569 (96%)	22 (4%)	30	65

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

Mol	Chain	Res	Type
1	A	16	LYS
1	A	26	VAL
1	A	123	VAL
1	A	141	SER
1	A	215	GLU
1	A	236	LEU
1	A	283	GLU
1	A	329	ARG
1	A	381	ILE
1	B	16	LYS

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Mol	Chain	Res	Type
1	B	26	VAL
1	B	44	ILE
1	B	94	THR
1	B	123	VAL
1	B	141	SER
1	B	239	GLN
1	B	283	GLU
1	B	290	MET
1	B	329	ARG
1	B	331	SER
1	B	339	ILE
1	B	400	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	151	GLN
1	A	238	GLN
1	A	348	GLN
1	A	371	GLN
1	B	11	ASN
1	B	151	GLN
1	B	230	GLN
1	B	348	GLN
1	B	371	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 oligosaccharides 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	B	501	-	4,4,4	0.26	0	6,6,6	0.29	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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	SO4	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	364/433 (84%)	1.33	101 (27%)  	11, 32, 69, 154	0
1	B	352/433 (81%)	1.21	80 (22%)  	12, 31, 69, 161	0
All	All	716/866 (82%)	1.27	181 (25%)  	11, 31, 70, 161	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	GLY	8.9
1	B	423	ALA	8.7
1	B	280	GLY	7.6
1	A	281	ASN	7.6
1	B	283	GLU	7.3
1	A	151	GLN	6.4
1	A	283	GLU	6.3
1	A	1	MET	6.2
1	B	281	ASN	6.1
1	A	148	ALA	5.7
1	B	358	LYS	5.3
1	A	380	GLU	5.2
1	B	284	GLU	5.1
1	A	282	GLY	5.0
1	A	285	GLY	5.0
1	A	149	LYS	5.0
1	A	284	GLU	5.0
1	B	148	ALA	4.9
1	B	375	GLU	4.9
1	A	421	LYS	4.8
1	A	215	GLU	4.7
1	A	150	GLU	4.7
1	B	151	GLN	4.7
1	A	288	MET	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	216	ASP	4.5
1	B	360	THR	4.4
1	B	356	ALA	4.4
1	A	147	GLU	4.4
1	B	380	GLU	4.4
1	A	418	CYS	4.3
1	A	52	GLU	4.3
1	A	328	SER	4.3
1	B	72	SER	4.3
1	B	347	ASP	4.3
1	B	222	ALA	4.3
1	A	424	ALA	4.2
1	A	376	GLU	4.2
1	B	418	CYS	4.1
1	B	420	ASP	4.0
1	A	347	ASP	4.0
1	B	355	PRO	4.0
1	A	213	GLU	4.0
1	B	421	LYS	4.0
1	A	422	LEU	3.9
1	B	147	GLU	3.9
1	B	149	LYS	3.9
1	A	419	VAL	3.9
1	B	282	GLY	3.9
1	B	377	THR	3.8
1	A	379	GLY	3.8
1	A	287	LEU	3.7
1	A	219	THR	3.7
1	A	212	ILE	3.7
1	A	230	GLN	3.6
1	A	378	ASP	3.6
1	A	420	ASP	3.6
1	B	306	GLU	3.6
1	A	44	ILE	3.5
1	B	42	GLU	3.5
1	A	286	GLY	3.4
1	B	400	THR	3.4
1	A	129	GLY	3.4
1	A	402	GLN	3.3
1	A	218	GLU	3.3
1	B	410	GLY	3.3
1	B	397	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	285	GLY	3.3
1	A	238	GLN	3.2
1	A	408	HIS	3.2
1	A	396	LYS	3.2
1	A	239	GLN	3.2
1	A	220	ILE	3.2
1	B	378	ASP	3.1
1	B	346	THR	3.1
1	B	409	ASP	3.1
1	A	360	THR	3.1
1	B	331	SER	3.1
1	A	410	GLY	3.1
1	A	423	ALA	3.0
1	B	53	SER	3.0
1	B	141	SER	3.0
1	A	94	THR	3.0
1	A	240	THR	3.0
1	B	240	THR	3.0
1	B	223	LYS	3.0
1	A	236	LEU	3.0
1	A	244	ASN	2.9
1	A	400	THR	2.9
1	B	104	GLU	2.9
1	A	30	TYR	2.8
1	A	375	GLU	2.8
1	B	74	ASP	2.8
1	B	71	GLU	2.8
1	A	357	GLY	2.8
1	B	75	SER	2.8
1	A	229	LEU	2.8
1	A	346	THR	2.8
1	A	358	LYS	2.7
1	A	377	THR	2.7
1	B	389	ARG	2.7
1	B	354	THR	2.7
1	B	243	ASP	2.7
1	B	239	GLN	2.7
1	B	150	GLU	2.7
1	B	376	GLU	2.7
1	A	32	CYS	2.7
1	A	356	ALA	2.7
1	B	31	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	389	ARG	2.6
1	B	238	GLN	2.6
1	B	20	ARG	2.6
1	B	224	ASP	2.6
1	A	241	GLY	2.6
1	A	361	GLU	2.6
1	B	246	GLU	2.6
1	A	98	ASP	2.6
1	B	51	ASP	2.6
1	B	381	ILE	2.5
1	A	97	ASP	2.5
1	A	359	PRO	2.5
1	A	233	ILE	2.5
1	B	41	GLU	2.5
1	A	349	THR	2.5
1	A	304	ASN	2.5
1	B	422	LEU	2.4
1	A	139	ALA	2.4
1	B	398	GLY	2.4
1	A	316	HIS	2.4
1	A	234	ASP	2.4
1	A	64	ARG	2.3
1	B	34	VAL	2.3
1	A	318	GLY	2.3
1	B	286	GLY	2.3
1	A	279	ALA	2.3
1	B	328	SER	2.3
1	B	359	PRO	2.3
1	A	289	GLY	2.3
1	B	357	GLY	2.3
1	B	379	GLY	2.3
1	A	131	ARG	2.3
1	A	71	GLU	2.3
1	A	214	LEU	2.3
1	B	260	ASP	2.3
1	B	396	LYS	2.3
1	A	127	PRO	2.3
1	A	72	SER	2.2
1	A	142	GLY	2.2
1	A	35	GLU	2.2
1	A	395	LYS	2.2
1	B	117	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	138	SER	2.2
1	B	411	TYR	2.2
1	B	327	GLY	2.2
1	B	52	GLU	2.2
1	B	384	ARG	2.2
1	A	336	ASP	2.2
1	B	349	THR	2.2
1	B	92	ALA	2.2
1	B	391	ARG	2.1
1	B	319	SER	2.1
1	A	243	ASP	2.1
1	A	398	GLY	2.1
1	A	102	PHE	2.1
1	B	27	ARG	2.1
1	A	417	ILE	2.1
1	B	278	GLN	2.1
1	A	221	HIS	2.1
1	A	249	LYS	2.1
1	A	415	PRO	2.1
1	A	224	ASP	2.1
1	A	245	ILE	2.1
1	A	27	ARG	2.1
1	A	324	TYR	2.1
1	A	31	LYS	2.0
1	B	394	LEU	2.0
1	A	384	ARG	2.0
1	B	361	GLU	2.0
1	A	317	VAL	2.0
1	A	291	LEU	2.0
1	B	413	ASN	2.0
1	B	414	ALA	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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	501	5/5	0.89	0.19	54,54,54,54	0

6.5 Other polymers

There are no such residues in this entry.