



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:30 PM UTC

PDB ID : 5JJ6 / pdb_00005jj6
Title : Fic-1 (aa134 - 508) from *C. elegans*
Authors : Cruz, V.E.; Schwartz, T.U.
Deposited on : 2016-04-22
Resolution : 2.91 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

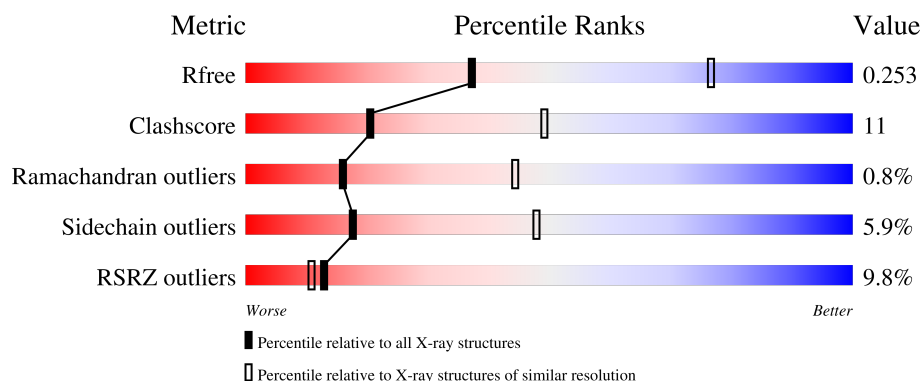
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	382	12% 62% 20% • 14%
1	B	382	5% 69% 17% • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5100 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 Adenosine monophosphate-protein transferase FICD homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2503	1573	454	462	14			
1	B	333	Total	C	N	O	S	0	0	0
			2581	1625	466	473	17			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	MET	-	initiating methionine	UNP Q23544
A	128	HIS	-	expression tag	UNP Q23544
A	129	HIS	-	expression tag	UNP Q23544
A	130	HIS	-	expression tag	UNP Q23544
A	131	HIS	-	expression tag	UNP Q23544
A	132	HIS	-	expression tag	UNP Q23544
A	133	HIS	-	expression tag	UNP Q23544
B	127	MET	-	initiating methionine	UNP Q23544
B	128	HIS	-	expression tag	UNP Q23544
B	129	HIS	-	expression tag	UNP Q23544
B	130	HIS	-	expression tag	UNP Q23544
B	131	HIS	-	expression tag	UNP Q23544
B	132	HIS	-	expression tag	UNP Q23544
B	133	HIS	-	expression tag	UNP Q23544

- 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		

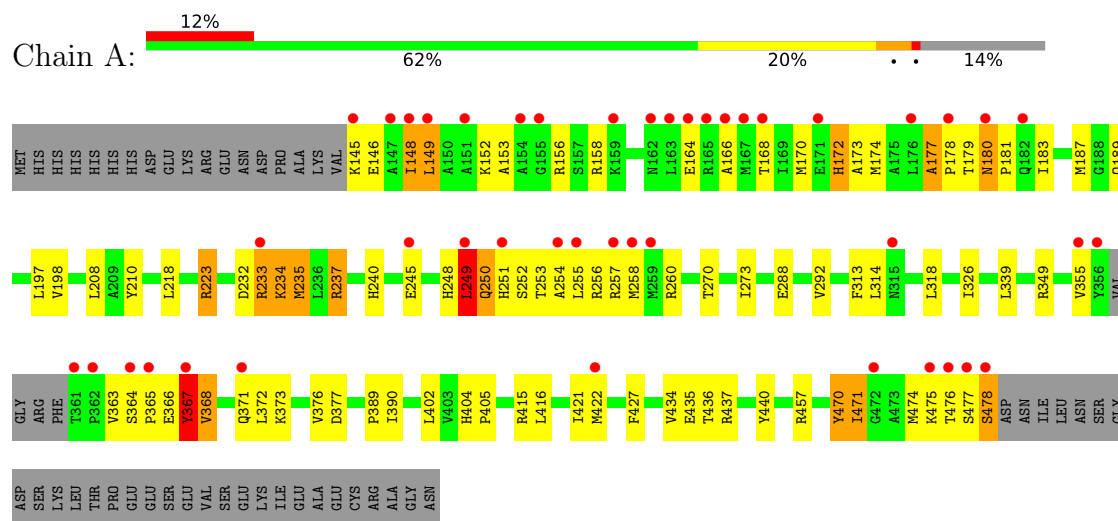
- Molecule 3 is water.

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

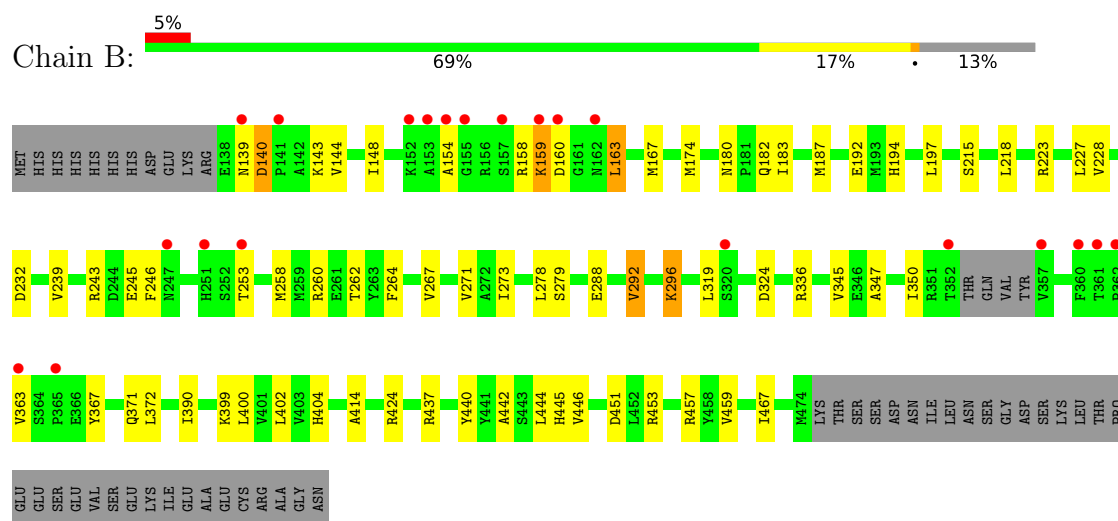
3 Residue-property plots

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: Adenosine monophosphate-protein transferase FICD homolog



- Molecule 1: Adenosine monophosphate-protein transferase FICD homolog



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	192.15Å 192.15Å 182.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	122.97 – 2.91 122.97 – 2.91	Depositor EDS
% Data completeness (in resolution range)	97.5 (122.97-2.91) 92.1 (122.97-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.206 , 0.255 0.214 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (6.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.0	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	0.93	EDS
Total number of atoms	5100	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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	0.59	1/2545 (0.0%)	1.06	15/3457 (0.4%)
1	B	0.58	0/2626	0.93	5/3557 (0.1%)
All	All	0.58	1/5171 (0.0%)	1.00	20/7014 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	ARG	CD-NE	6.00	1.54	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	MET	N-CA-C	-8.93	101.52	111.07
1	A	368	VAL	N-CA-C	7.74	118.54	110.72
1	A	233	ARG	CA-C-N	-7.68	110.62	122.60
1	A	233	ARG	C-N-CA	-7.68	110.62	122.60
1	A	421	ILE	N-CA-C	7.54	118.28	110.36
1	A	149	LEU	N-CA-C	-6.96	103.46	112.23
1	A	177	ALA	CA-C-N	6.81	128.35	119.84
1	A	177	ALA	C-N-CA	6.81	128.35	119.84
1	A	254	ALA	N-CA-C	-6.25	104.57	111.82
1	B	404	HIS	CA-C-N	6.20	126.73	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	HIS	C-N-CA	6.20	126.73	120.04
1	A	249	LEU	CA-CB-CG	5.86	136.82	116.30
1	A	180	ASN	CA-C-N	5.59	125.26	119.05
1	A	180	ASN	C-N-CA	5.59	125.26	119.05
1	A	152	LYS	N-CA-C	-5.44	105.90	112.54
1	A	367	TYR	N-CA-C	-5.41	106.99	113.21
1	B	140	ASP	CA-C-N	-5.35	114.44	119.85
1	B	140	ASP	C-N-CA	-5.35	114.44	119.85
1	A	172	HIS	N-CA-C	-5.27	105.65	111.71
1	B	167	MET	N-CA-C	5.02	116.45	110.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	367	TYR	Peptide

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	2503	0	2470	80	0
1	B	2581	0	2575	35	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
All	All	5100	0	5045	114	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 11.

All (114) 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:257:ARG:NH2	1:A:474:MET:SD	2.29	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:MET:HE1	1:A:470:TYR:CD2	2.00	0.97
1:A:258:MET:SD	1:A:470:TYR:CE2	2.58	0.96
1:A:234:LYS:HB2	1:A:237:ARG:HD2	1.56	0.88
1:A:223:ARG:HH11	1:A:223:ARG:CB	1.89	0.85
1:A:148:ILE:HD13	1:A:172:HIS:HE1	1.41	0.85
1:A:258:MET:SD	1:A:470:TYR:CD2	2.70	0.84
1:A:258:MET:CE	1:A:470:TYR:CD2	2.64	0.81
1:A:363:VAL:HG21	1:A:404:HIS:HB3	1.61	0.80
1:A:390:ILE:HG12	1:A:422:MET:HE3	1.67	0.75
1:A:148:ILE:HG12	1:A:173:ALA:HA	1.67	0.75
1:A:177:ALA:HB1	1:A:183:ILE:HD13	1.69	0.74
1:A:258:MET:HE1	1:A:470:TYR:HD2	1.53	0.73
1:A:148:ILE:HD13	1:A:172:HIS:CE1	2.23	0.72
1:A:232:ASP:OD2	1:A:457:ARG:NH1	2.23	0.72
1:A:248:HIS:O	1:A:249:LEU:HB3	1.92	0.69
1:A:223:ARG:HH11	1:A:223:ARG:CG	2.06	0.68
1:B:192:GLU:OE1	1:B:223:ARG:NH2	2.26	0.68
1:B:215:SER:HA	1:B:218:LEU:HD12	1.76	0.67
1:B:144:VAL:HG13	1:B:183:ILE:HD11	1.77	0.67
1:A:223:ARG:HH11	1:A:223:ARG:HB3	1.60	0.64
1:B:163:LEU:CB	1:B:194:HIS:NE2	2.62	0.62
1:A:234:LYS:O	1:A:234:LYS:HG3	2.00	0.62
1:A:253:THR:HA	1:A:256:ARG:HB3	1.82	0.62
1:A:174:MET:HG3	1:A:187:MET:HE3	1.80	0.61
1:A:270:THR:HG23	1:A:415:ARG:HH11	1.64	0.61
1:B:158:ARG:HG3	1:B:159:LYS:H	1.66	0.60
1:A:234:LYS:CG	1:A:237:ARG:HB2	2.32	0.60
1:B:446:VAL:HG12	1:B:451:ASP:HB3	1.83	0.59
1:A:245:GLU:HG2	1:A:248:HIS:CE1	2.38	0.58
1:A:292:VAL:HG11	1:B:292:VAL:HG13	1.84	0.58
1:A:368:VAL:HA	1:A:371:GLN:OE1	2.04	0.58
1:A:234:LYS:HA	1:A:237:ARG:H	1.69	0.58
1:A:245:GLU:HA	1:A:248:HIS:CE1	2.40	0.57
1:A:252:SER:HA	1:A:255:LEU:HD13	1.87	0.56
1:B:246:PHE:HB2	1:B:467:ILE:HG23	1.88	0.55
1:A:245:GLU:HG2	1:A:248:HIS:HE1	1.73	0.54
1:A:470:TYR:CD1	1:A:470:TYR:N	2.73	0.54
1:A:257:ARG:HH11	1:A:470:TYR:HB3	1.72	0.54
1:A:258:MET:CE	1:A:470:TYR:HD2	2.10	0.54
1:A:148:ILE:HD11	1:A:173:ALA:HB2	1.91	0.53
1:A:164:GLU:O	1:A:168:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:HA	1:A:149:LEU:HG	1.92	0.51
1:A:476:THR:C	1:A:478:SER:H	2.19	0.51
1:A:250:GLN:CD	1:A:250:GLN:H	2.17	0.50
1:A:234:LYS:HE2	1:A:237:ARG:HD2	1.93	0.50
1:A:314:LEU:HA	1:A:318:LEU:HD13	1.93	0.50
1:A:326:ILE:O	1:A:376:VAL:HG13	2.11	0.50
1:A:234:LYS:CB	1:A:237:ARG:HB2	2.42	0.49
1:A:233:ARG:O	1:A:237:ARG:HG3	2.11	0.49
1:A:252:SER:O	1:A:255:LEU:HB2	2.12	0.49
1:A:158:ARG:O	1:A:166:ALA:HB2	2.12	0.49
1:A:260:ARG:NH2	1:A:288:GLU:OE2	2.42	0.49
1:A:273:ILE:HA	1:A:434:VAL:HG23	1.95	0.49
1:A:153:ALA:C	1:A:156:ARG:H	2.20	0.49
1:B:197:LEU:HD21	1:B:227:LEU:HD13	1.94	0.49
1:A:422:MET:O	1:A:427:PHE:HB2	2.13	0.48
1:A:372:LEU:HD11	1:A:405:PRO:HB3	1.94	0.48
1:A:476:THR:C	1:A:478:SER:N	2.69	0.48
1:A:234:LYS:HG3	1:A:237:ARG:HB2	1.95	0.48
1:A:470:TYR:N	1:A:470:TYR:HD1	2.09	0.48
1:A:363:VAL:HG23	1:A:402:LEU:O	2.13	0.48
1:B:239:VAL:HG11	1:B:390:ILE:HD11	1.96	0.47
1:A:148:ILE:HG13	1:A:148:ILE:O	2.13	0.47
1:B:336:ARG:HA	1:B:347:ALA:HB1	1.96	0.47
1:A:146:GLU:CB	1:A:149:LEU:HG	2.45	0.47
1:B:148:ILE:HG21	1:B:182:GLN:OE1	2.13	0.47
1:B:264:PHE:CZ	1:B:288:GLU:HB2	2.50	0.46
1:A:223:ARG:HB3	1:A:223:ARG:NH1	2.29	0.46
1:A:470:TYR:O	1:A:471:ILE:C	2.56	0.46
1:B:437:ARG:O	1:B:440:TYR:HB3	2.15	0.46
1:A:208:LEU:HD21	1:A:218:LEU:HG	1.98	0.45
1:B:192:GLU:CD	1:B:223:ARG:HH22	2.25	0.45
1:B:267:VAL:O	1:B:271:VAL:HG22	2.17	0.45
1:B:278:LEU:HD23	1:B:296:LYS:HE3	1.98	0.44
1:B:367:TYR:O	1:B:371:GLN:HG3	2.18	0.44
1:A:240:HIS:CE1	1:A:389:PRO:HD2	2.52	0.44
1:B:399:LYS:HB3	1:B:399:LYS:HE2	1.86	0.44
1:A:245:GLU:O	1:A:245:GLU:CD	2.60	0.44
1:B:180:ASN:HB3	1:B:183:ILE:HD12	2.00	0.44
1:A:234:LYS:O	1:A:234:LYS:CG	2.64	0.43
1:B:158:ARG:HG3	1:B:159:LYS:N	2.31	0.43
1:A:180:ASN:HA	1:A:181:PRO:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ALA:O	1:B:445:HIS:HB3	2.19	0.43
1:A:179:THR:HG22	1:A:210:TYR:CE2	2.54	0.43
1:B:243:ARG:HA	1:B:467:ILE:HD13	2.01	0.43
1:B:400:LEU:HD23	1:B:414:ALA:HA	2.01	0.42
1:A:235:MET:HE2	1:A:235:MET:HB3	1.86	0.42
1:B:319:LEU:HD22	1:B:424:ARG:HG2	2.02	0.42
1:A:170:MET:O	1:A:173:ALA:HB3	2.18	0.42
1:A:367:TYR:C	1:A:371:GLN:HE22	2.28	0.42
1:A:177:ALA:CB	1:A:183:ILE:HD13	2.43	0.42
1:A:363:VAL:HG21	1:A:404:HIS:CB	2.43	0.42
1:A:364:SER:HA	1:A:365:PRO:HD3	1.97	0.41
1:A:416:LEU:HD23	1:A:416:LEU:HA	1.92	0.41
1:B:260:ARG:HD3	1:B:260:ARG:HA	1.57	0.41
1:A:148:ILE:O	1:A:148:ILE:CG1	2.69	0.41
1:A:437:ARG:O	1:A:440:TYR:HB3	2.21	0.41
1:B:159:LYS:HE2	1:B:159:LYS:HB3	1.81	0.41
1:B:444:LEU:HA	1:B:444:LEU:HD23	1.82	0.41
1:B:232:ASP:OD2	1:B:457:ARG:NH1	2.54	0.41
1:B:228:VAL:HG21	1:B:453:ARG:NH1	2.36	0.41
1:A:145:LYS:HA	1:A:145:LYS:HD3	1.69	0.41
1:B:139:ASN:OD1	1:B:140:ASP:O	2.38	0.41
1:A:249:LEU:HD12	1:A:251:HIS:H	1.86	0.41
1:B:372:LEU:HD23	1:B:372:LEU:HA	1.74	0.41
1:A:435:GLU:HG2	1:A:436:THR:HG23	2.03	0.40
1:A:146:GLU:CA	1:A:149:LEU:HG	2.50	0.40
1:B:174:MET:HG3	1:B:187:MET:HE3	2.04	0.40
1:B:215:SER:HA	1:B:218:LEU:HB2	2.03	0.40
1:A:313:PHE:CE2	1:A:318:LEU:HD11	2.56	0.40
1:A:373:LYS:HG2	1:A:377:ASP:OD2	2.21	0.40
1:A:223:ARG:HH11	1:A:223:ARG:HG3	1.86	0.40
1:B:160:ASP:O	1:B:160:ASP:OD1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	326/382 (85%)	308 (94%)	16 (5%)	2 (1%)	21	51
1	B	329/382 (86%)	313 (95%)	13 (4%)	3 (1%)	14	41
All	All	655/764 (86%)	621 (95%)	29 (4%)	5 (1%)	16	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	LEU
1	A	178	PRO
1	B	154	ALA
1	B	324	ASP
1	A	366	GLU

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	257/328 (78%)	241 (94%)	16 (6%)	16	46
1	B	269/328 (82%)	254 (94%)	15 (6%)	19	50
All	All	526/656 (80%)	495 (94%)	31 (6%)	18	48

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ILE
1	A	189	GLN
1	A	197	LEU
1	A	198	VAL
1	A	223	ARG
1	A	234	LYS
1	A	249	LEU
1	A	250	GLN

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Mol	Chain	Res	Type
1	A	339	LEU
1	A	349	ARG
1	A	355	VAL
1	A	470	TYR
1	A	471	ILE
1	A	475	LYS
1	A	477	SER
1	A	478	SER
1	B	143	LYS
1	B	159	LYS
1	B	245	GLU
1	B	253	THR
1	B	258	MET
1	B	262	THR
1	B	273	ILE
1	B	279	SER
1	B	292	VAL
1	B	296	LYS
1	B	345	VAL
1	B	350	ILE
1	B	363	VAL
1	B	402	LEU
1	B	459	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	HIS
1	B	247	ASN
1	B	445	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	601	-	4,4,4	0.38	0	6,6,6	0.62	0
2	SO4	A	601	-	4,4,4	0.29	0	6,6,6	0.18	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.

No monomer is involved in short contacts.

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	330/382 (86%)	0.63	44 (13%) 7 6	27, 71, 134, 144	0
1	B	333/382 (87%)	0.22	21 (6%) 26 20	30, 52, 105, 138	0
All	All	663/764 (86%)	0.42	65 (9%) 13 11	27, 61, 127, 144	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	MET	7.6
1	B	155	GLY	5.4
1	A	475	LYS	4.8
1	A	476	THR	4.8
1	A	147	ALA	4.6
1	B	357	VAL	4.5
1	A	478	SER	4.5
1	B	352	THR	4.4
1	B	162	ASN	4.2
1	A	255	LEU	4.1
1	A	145	LYS	3.8
1	A	367	TYR	3.6
1	A	148	ILE	3.6
1	A	251	HIS	3.6
1	A	477	SER	3.5
1	B	139	ASN	3.5
1	A	364	SER	3.4
1	B	159	LYS	3.4
1	A	249	LEU	3.3
1	A	362	PRO	3.3
1	A	365	PRO	3.2
1	A	159	LYS	3.2
1	A	257	ARG	3.2
1	A	162	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	3.1
1	B	363	VAL	3.0
1	A	178	PRO	2.9
1	A	180	ASN	2.8
1	A	171	GLU	2.7
1	A	371	GLN	2.7
1	B	154	ALA	2.7
1	B	360	PHE	2.7
1	A	164	GLU	2.6
1	A	356	TYR	2.6
1	B	153	ALA	2.6
1	A	154	ALA	2.6
1	A	472	GLY	2.4
1	B	320	SER	2.4
1	B	361	THR	2.4
1	A	167	MET	2.4
1	A	315	ASN	2.4
1	A	182	GLN	2.3
1	B	152	LYS	2.3
1	A	149	LEU	2.3
1	B	251	HIS	2.3
1	A	355	VAL	2.3
1	A	254	ALA	2.3
1	A	233	ARG	2.3
1	B	365	PRO	2.3
1	A	155	GLY	2.3
1	A	168	THR	2.2
1	B	157	SER	2.2
1	A	258	MET	2.2
1	A	361	THR	2.2
1	A	165	ARG	2.2
1	B	253	THR	2.2
1	A	151	ALA	2.2
1	A	176	LEU	2.1
1	A	245	GLU	2.1
1	B	247	ASN	2.1
1	B	362	PRO	2.1
1	A	166	ALA	2.1
1	B	160	ASP	2.1
1	B	141	PRO	2.0
1	A	422	MET	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	A	601	5/5	0.91	0.12	54,57,80,80	0
2	SO4	B	601	5/5	0.94	0.12	40,44,49,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.