



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:52 AM UTC

PDB ID : 4IGP / pdb_00004igp
Title : Histone H3 Lysine 4 Demethylating Rice JMJ703 apo enzyme
Authors : Chen, Q.F.; Chen, X.S.; Wang, Q.; Zhang, F.B.; Lou, Z.Y.; Zhang, Q.F.;
Zhou, D.X.
Deposited on : 2012-12-17
Resolution : 3.00 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
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

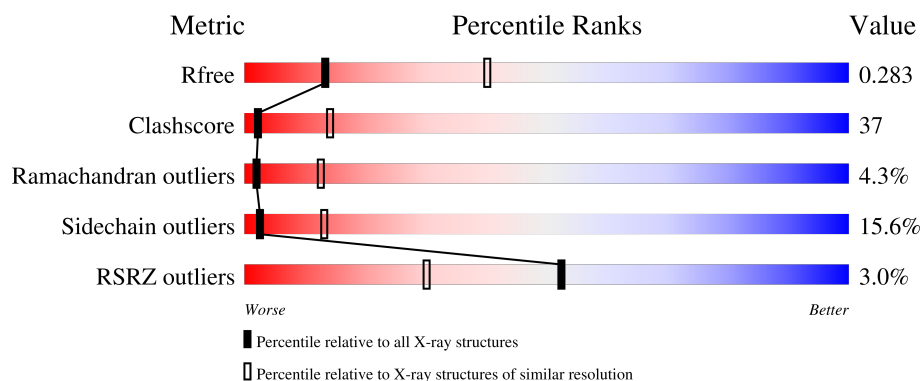
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	360	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2209 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 Os05g0196500 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2208	1434	363	401	10			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 1: Os05g0196500 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	91.33Å 91.33Å 76.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.66 – 3.00 45.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.8 (45.66-3.00) 90.6 (45.66-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.227 , 0.287 0.227 , 0.283	Depositor DCC
R_{free} test set	321 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2209	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: FE

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	0.66	0/2280	1.21	25/3099 (0.8%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	436	LEU	N-CA-CB	-16.80	84.25	110.28
1	A	351	GLN	CB-CA-C	-10.43	90.28	110.10
1	A	148	ARG	CA-C-N	8.17	128.48	119.90
1	A	148	ARG	C-N-CA	8.17	128.48	119.90
1	A	352	SER	N-CA-C	-7.21	98.19	109.72
1	A	379	VAL	CA-C-N	7.08	128.93	120.23
1	A	379	VAL	C-N-CA	7.08	128.93	120.23
1	A	351	GLN	N-CA-C	7.04	130.70	111.00
1	A	435	GLU	CB-CA-C	6.79	123.93	110.42
1	A	188	PRO	O-C-N	6.75	124.32	121.15
1	A	140	LYS	N-CA-C	6.44	118.88	108.32
1	A	142	ASN	CA-C-N	6.33	125.90	119.19
1	A	142	ASN	C-N-CA	6.33	125.90	119.19
1	A	322	GLY	N-CA-C	-6.24	102.55	112.66
1	A	187	VAL	CA-C-N	6.19	124.12	119.66
1	A	187	VAL	C-N-CA	6.19	124.12	119.66
1	A	410	ALA	CA-C-N	5.93	125.95	119.90
1	A	410	ALA	C-N-CA	5.93	125.95	119.90
1	A	466	CYS	N-CA-C	5.89	117.48	108.52
1	A	452	SER	CA-C-N	5.72	125.33	119.56
1	A	452	SER	C-N-CA	5.72	125.33	119.56
1	A	203	ILE	N-CA-C	-5.65	104.03	111.09
1	A	436	LEU	N-CA-C	5.31	117.98	111.82
1	A	302	ILE	CB-CA-C	-5.28	105.20	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	HIS	N-CA-C	-5.23	105.19	112.30

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	2208	0	2089	157	0
2	A	1	0	0	0	0
All	All	2209	0	2089	157	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 37.

All (157) 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:361:ARG:HG3	1:A:361:ARG:HH11	1.00	1.16
1:A:429:MET:HE2	1:A:451:PHE:HB2	1.39	1.02
1:A:435:GLU:O	1:A:438:GLU:HB2	1.62	0.99
1:A:361:ARG:HG3	1:A:361:ARG:NH1	1.76	0.95
1:A:275:PHE:HE1	1:A:320:ILE:HG22	1.33	0.91
1:A:148:ARG:HE	1:A:300:GLU:HG3	1.34	0.90
1:A:212:ARG:NH1	1:A:264:PHE:O	2.05	0.88
1:A:323:ALA:H	1:A:325:LEU:HD21	1.38	0.87
1:A:437:PHE:HE1	1:A:444:LEU:HD11	1.36	0.87
1:A:352:SER:HB3	1:A:354:TRP:HD1	1.40	0.86
1:A:350:ALA:N	1:A:351:GLN:HB2	1.93	0.83
1:A:361:ARG:HH11	1:A:361:ARG:CG	1.89	0.83
1:A:399:HIS:O	1:A:478:PRO:HB3	1.80	0.81
1:A:170:TYR:O	1:A:173:SER:HB3	1.81	0.80
1:A:423:VAL:O	1:A:427:SER:HB3	1.81	0.79
1:A:429:MET:HE2	1:A:451:PHE:CB	2.13	0.79
1:A:424:ASN:HB3	1:A:461:VAL:HG22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:SER:HB3	1:A:354:TRP:CD1	2.19	0.77
1:A:437:PHE:CE1	1:A:444:LEU:HD11	2.20	0.76
1:A:431:LYS:NZ	1:A:459:GLU:CD	2.46	0.74
1:A:392:CYS:HA	1:A:450:GLN:OE1	1.89	0.72
1:A:322:GLY:O	1:A:323:ALA:HB2	1.92	0.69
1:A:409:GLY:HA3	1:A:490:ASN:HA	1.75	0.68
1:A:163:GLU:HB3	1:A:170:TYR:CD1	2.29	0.68
1:A:275:PHE:HE1	1:A:320:ILE:CG2	2.06	0.67
1:A:357:ASN:HA	1:A:380:PRO:HG2	1.75	0.67
1:A:162:GLU:O	1:A:165:GLU:HG2	1.94	0.67
1:A:275:PHE:CE1	1:A:320:ILE:HG22	2.22	0.66
1:A:166:ASP:OD2	1:A:169:LYS:NZ	2.29	0.65
1:A:437:PHE:HE1	1:A:444:LEU:CD1	2.09	0.65
1:A:431:LYS:HZ2	1:A:459:GLU:CD	2.05	0.65
1:A:162:GLU:H	1:A:162:GLU:CD	2.02	0.64
1:A:211:THR:HB	1:A:320:ILE:HG23	1.80	0.63
1:A:440:GLN:O	1:A:442:ASP:N	2.31	0.63
1:A:163:GLU:O	1:A:170:TYR:HB2	1.99	0.63
1:A:352:SER:CB	1:A:354:TRP:HD1	2.10	0.63
1:A:350:ALA:CA	1:A:351:GLN:HB2	2.29	0.62
1:A:319:VAL:HG13	1:A:386:MET:SD	2.39	0.62
1:A:148:ARG:HE	1:A:300:GLU:CG	2.11	0.62
1:A:431:LYS:NZ	1:A:459:GLU:OE1	2.32	0.61
1:A:404:ASN:O	1:A:473:PHE:HA	2.01	0.61
1:A:164:PHE:HE2	1:A:192:TRP:CD1	2.18	0.60
1:A:213:VAL:HG22	1:A:320:ILE:HD11	1.83	0.60
1:A:187:VAL:HG22	1:A:472:GLU:HG2	1.82	0.60
1:A:465:ARG:O	1:A:466:CYS:HB3	2.01	0.60
1:A:168:LEU:HD21	1:A:362:LEU:HB2	1.83	0.60
1:A:394:HIS:HE1	1:A:396:GLU:OE2	1.84	0.59
1:A:396:GLU:OE2	1:A:482:HIS:CE1	2.55	0.59
1:A:406:MET:HA	1:A:406:MET:HE3	1.85	0.59
1:A:204:TRP:HE1	1:A:273:GLN:HG3	1.67	0.59
1:A:443:LEU:O	1:A:446:ASN:HB2	2.03	0.58
1:A:305:GLU:O	1:A:308:ARG:HB3	2.03	0.58
1:A:315:GLU:HG2	1:A:317:ILE:HD12	1.84	0.58
1:A:275:PHE:CE2	1:A:384:VAL:HG12	2.38	0.58
1:A:439:GLU:HG3	1:A:440:GLN:HG3	1.84	0.58
1:A:163:GLU:HB3	1:A:170:TYR:HD1	1.67	0.58
1:A:426:GLU:HB3	1:A:444:LEU:CD2	2.35	0.57
1:A:215:LYS:HE2	1:A:316:GLU:OE2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:TYR:HD1	1:A:322:GLY:O	1.89	0.56
1:A:393:TRP:HD1	1:A:451:PHE:H	1.52	0.56
1:A:392:CYS:HB3	1:A:449:THR:O	2.06	0.56
1:A:410:ALA:HB1	1:A:411:PRO:HD2	1.87	0.56
1:A:316:GLU:HG3	1:A:317:ILE:N	2.19	0.56
1:A:302:ILE:O	1:A:305:GLU:N	2.38	0.55
1:A:311:GLU:HB2	1:A:312:VAL:HG23	1.89	0.55
1:A:400:LEU:HG	1:A:496:ASN:HB3	1.89	0.55
1:A:393:TRP:CD1	1:A:451:PHE:H	2.24	0.54
1:A:446:ASN:O	1:A:447:LEU:HB2	2.05	0.54
1:A:154:ALA:HB3	1:A:466:CYS:HB3	1.90	0.54
1:A:396:GLU:OE1	1:A:396:GLU:HA	2.08	0.53
1:A:148:ARG:NE	1:A:300:GLU:HG3	2.15	0.53
1:A:215:LYS:O	1:A:216:VAL:C	2.51	0.53
1:A:398:HIS:C	1:A:399:HIS:ND1	2.67	0.53
1:A:276:GLN:HG3	1:A:489:PHE:CD2	2.44	0.52
1:A:178:ALA:HB3	1:A:477:PHE:CZ	2.44	0.52
1:A:311:GLU:C	1:A:312:VAL:CG2	2.83	0.52
1:A:179:GLU:N	1:A:180:PRO:CD	2.72	0.52
1:A:350:ALA:N	1:A:352:SER:N	2.57	0.52
1:A:315:GLU:HG2	1:A:317:ILE:CD1	2.39	0.52
1:A:405:TYR:HB2	1:A:473:PHE:CE2	2.46	0.51
1:A:217:ASP:HB2	1:A:313:PRO:HB3	1.93	0.51
1:A:167:THR:HA	1:A:354:TRP:CZ2	2.46	0.51
1:A:406:MET:HA	1:A:406:MET:CE	2.41	0.50
1:A:178:ALA:HB3	1:A:477:PHE:HZ	1.76	0.49
1:A:200:ASP:OD1	1:A:201:LYS:N	2.45	0.49
1:A:356:LEU:HB3	1:A:495:VAL:CG2	2.42	0.49
1:A:425:LEU:C	1:A:425:LEU:HD13	2.37	0.49
1:A:264:PHE:HD1	1:A:321:TYR:HH	1.58	0.49
1:A:167:THR:HG1	1:A:354:TRP:CD1	2.30	0.49
1:A:434:PRO:O	1:A:435:GLU:C	2.56	0.49
1:A:322:GLY:O	1:A:323:ALA:CB	2.57	0.48
1:A:161:GLU:OE2	1:A:191:SER:HB3	2.13	0.48
1:A:451:PHE:CZ	1:A:455:LEU:HD23	2.48	0.48
1:A:391:PHE:CZ	1:A:412:LYS:HD3	2.49	0.48
1:A:303:GLU:HA	1:A:485:PHE:HZ	1.78	0.47
1:A:399:HIS:ND1	1:A:399:HIS:N	2.62	0.47
1:A:469:HIS:N	1:A:472:GLU:OE1	2.40	0.47
1:A:394:HIS:HE1	1:A:396:GLU:CD	2.22	0.47
1:A:305:GLU:HA	1:A:305:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HD22	1:A:443:LEU:HD11	1.97	0.47
1:A:444:LEU:H	1:A:444:LEU:HD12	1.80	0.47
1:A:359:LEU:O	1:A:360:PRO:C	2.58	0.46
1:A:426:GLU:HB3	1:A:444:LEU:HD22	1.98	0.46
1:A:278:TYR:C	1:A:278:TYR:CD1	2.93	0.45
1:A:440:GLN:C	1:A:442:ASP:H	2.25	0.45
1:A:359:LEU:O	1:A:361:ARG:N	2.50	0.45
1:A:414:TRP:NE1	1:A:474:VAL:HG21	2.31	0.45
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.69	0.45
1:A:214:GLN:HG3	1:A:321:TYR:HE2	1.82	0.45
1:A:214:GLN:NE2	1:A:321:TYR:CE2	2.85	0.45
1:A:162:GLU:C	1:A:164:PHE:N	2.74	0.44
1:A:350:ALA:HB3	1:A:351:GLN:HB2	2.00	0.44
1:A:406:MET:CE	1:A:492:ALA:HB2	2.48	0.44
1:A:402:SER:OG	1:A:476:THR:HB	2.18	0.44
1:A:477:PHE:O	1:A:480:ALA:HB3	2.17	0.44
1:A:408:TRP:HA	1:A:470:GLU:HG3	1.99	0.43
1:A:282:PHE:CD2	1:A:282:PHE:C	2.96	0.43
1:A:379:VAL:HG13	1:A:381:TRP:CD1	2.53	0.43
1:A:162:GLU:CD	1:A:162:GLU:N	2.74	0.43
1:A:323:ALA:O	1:A:324:ASP:HB2	2.19	0.43
1:A:270:PHE:HB3	1:A:275:PHE:HB2	2.00	0.43
1:A:302:ILE:O	1:A:303:GLU:C	2.62	0.43
1:A:413:LEU:HA	1:A:413:LEU:HD13	1.57	0.43
1:A:192:TRP:HZ3	1:A:405:TYR:OH	2.01	0.43
1:A:178:ALA:CB	1:A:477:PHE:CZ	3.02	0.43
1:A:417:VAL:HA	1:A:418:PRO:HD3	1.86	0.43
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.72	0.42
1:A:148:ARG:HA	1:A:149:PRO:HD3	1.63	0.42
1:A:201:LYS:O	1:A:201:LYS:HD3	2.19	0.42
1:A:145:GLY:O	1:A:147:ARG:HG3	2.19	0.42
1:A:223:LYS:HB3	1:A:223:LYS:HE2	1.80	0.42
1:A:425:LEU:HD22	1:A:456:LEU:HD21	2.00	0.42
1:A:400:LEU:HD12	1:A:497:VAL:C	2.44	0.42
1:A:268:PRO:HB2	1:A:270:PHE:CE2	2.54	0.42
1:A:359:LEU:N	1:A:360:PRO:HD2	2.34	0.42
1:A:426:GLU:HB3	1:A:444:LEU:HD21	2.01	0.42
1:A:142:ASN:HA	1:A:143:PRO:HD3	1.72	0.42
1:A:319:VAL:CG1	1:A:320:ILE:N	2.82	0.42
1:A:319:VAL:HG12	1:A:320:ILE:N	2.34	0.42
1:A:325:LEU:HD12	1:A:382:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:VAL:HA	1:A:188:PRO:HD3	1.83	0.42
1:A:325:LEU:H	1:A:325:LEU:HG	1.61	0.41
1:A:420:LYS:HB3	1:A:420:LYS:HE2	1.83	0.41
1:A:440:GLN:C	1:A:442:ASP:N	2.78	0.41
1:A:160:THR:OG1	1:A:163:GLU:HG3	2.20	0.41
1:A:162:GLU:C	1:A:164:PHE:H	2.27	0.41
1:A:167:THR:O	1:A:168:LEU:C	2.61	0.41
1:A:174:ILE:O	1:A:175:ARG:C	2.63	0.41
1:A:387:CYS:O	1:A:388:PHE:HB2	2.21	0.41
1:A:200:ASP:HB3	1:A:203:ILE:CD1	2.51	0.41
1:A:307:TRP:O	1:A:308:ARG:C	2.63	0.41
1:A:358:ASN:O	1:A:361:ARG:HG2	2.21	0.41
1:A:379:VAL:HA	1:A:380:PRO:HD3	1.75	0.41
1:A:404:ASN:N	1:A:404:ASN:ND2	2.68	0.40
1:A:490:ASN:OD1	1:A:490:ASN:C	2.63	0.40
1:A:273:GLN:HG2	1:A:277:LYS:HE2	2.03	0.40
1:A:311:GLU:C	1:A:312:VAL:HG23	2.47	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	258/360 (72%)	223 (86%)	24 (9%)	11 (4%)	2 12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	TRP
1	A	435	GLU
1	A	202	SER
1	A	323	ALA

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Mol	Chain	Res	Type
1	A	361	ARG
1	A	497	VAL
1	A	356	LEU
1	A	360	PRO
1	A	434	PRO
1	A	441	PRO
1	A	397	ASP

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	237/313 (76%)	200 (84%)	37 (16%)	2	13

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
1	A	169	LYS
1	A	175	ARG
1	A	177	MET
1	A	217	ASP
1	A	284	LYS
1	A	310	VAL
1	A	312	VAL
1	A	315	GLU
1	A	316	GLU
1	A	317	ILE
1	A	320	ILE
1	A	325	LEU
1	A	361	ARG
1	A	362	LEU
1	A	378	LEU
1	A	382	VAL
1	A	390	SER
1	A	399	HIS

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Mol	Chain	Res	Type
1	A	400	LEU
1	A	404	ASN
1	A	406	MET
1	A	408	TRP
1	A	413	LEU
1	A	420	LYS
1	A	425	LEU
1	A	426	GLU
1	A	427	SER
1	A	435	GLU
1	A	436	LEU
1	A	447	LEU
1	A	458	SER
1	A	463	VAL
1	A	476	THR
1	A	486	ASN
1	A	495	VAL
1	A	497	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	394	HIS
1	A	424	ASN
1	A	446	ASN

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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	270/360 (75%)	0.30	8 (2%) 52 30	20, 34, 71, 87	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	GLU	2.7
1	A	459	GLU	2.5
1	A	440	GLN	2.4
1	A	360	PRO	2.4
1	A	435	GLU	2.2
1	A	194	PRO	2.1
1	A	408	TRP	2.1
1	A	177	MET	2.1

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	FE	A	1000	1/1	0.98	0.08	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.