



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:54 PM UTC

PDB ID : 2ZIW / pdb_00002ziw
Title : Crystal structure of the Mus81-Eme1 complex
Authors : Chang, J.H.; Kim, J.J.; Choi, J.M.; Lee, J.H.; Cho, Y.
Deposited on : 2008-02-25
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

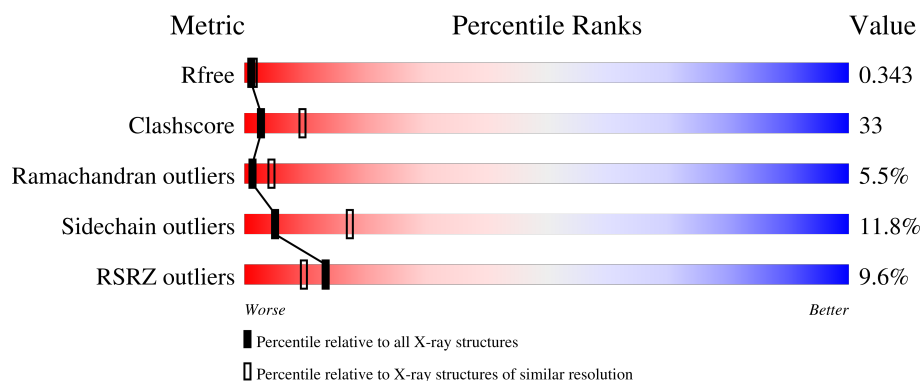
1 Overall quality at a glance

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	311	5% 42% 32% 11% • 13%
2	B	341	9% 32% 26% 8% • 33%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3869 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 Mus81 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	Se	0	0	0
			2155	1368	373	399	11	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	MSE	-	initiating methionine	UNP Q6GML8

- Molecule 2 is a protein called Crossover junction endonuclease EME1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	228	Total	C	N	O	S	Se	0	0	0
			1714	1079	304	321	6	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	230	MSE	-	expression tag	UNP Q96AY2
B	231	GLY	-	expression tag	UNP Q96AY2
B	232	SER	-	expression tag	UNP Q96AY2
B	233	SER	-	expression tag	UNP Q96AY2
B	234	HIS	-	expression tag	UNP Q96AY2
B	235	HIS	-	expression tag	UNP Q96AY2
B	236	HIS	-	expression tag	UNP Q96AY2
B	237	HIS	-	expression tag	UNP Q96AY2
B	238	HIS	-	expression tag	UNP Q96AY2
B	239	HIS	-	expression tag	UNP Q96AY2
B	240	SER	-	expression tag	UNP Q96AY2
B	241	GLN	-	expression tag	UNP Q96AY2
B	242	ASP	-	expression tag	UNP Q96AY2
B	243	PRO	-	expression tag	UNP Q96AY2
B	244	ASN	-	expression tag	UNP Q96AY2

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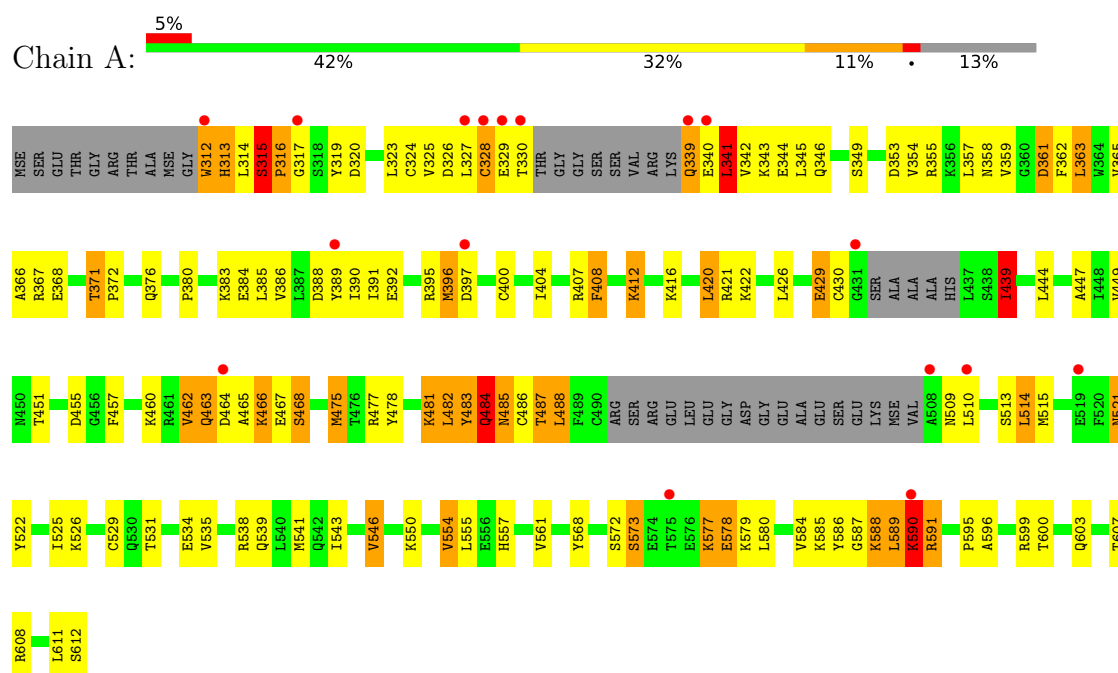
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Chain	Residue	Modelled	Actual	Comment	Reference
B	245	SER	-	expression tag	UNP Q96AY2

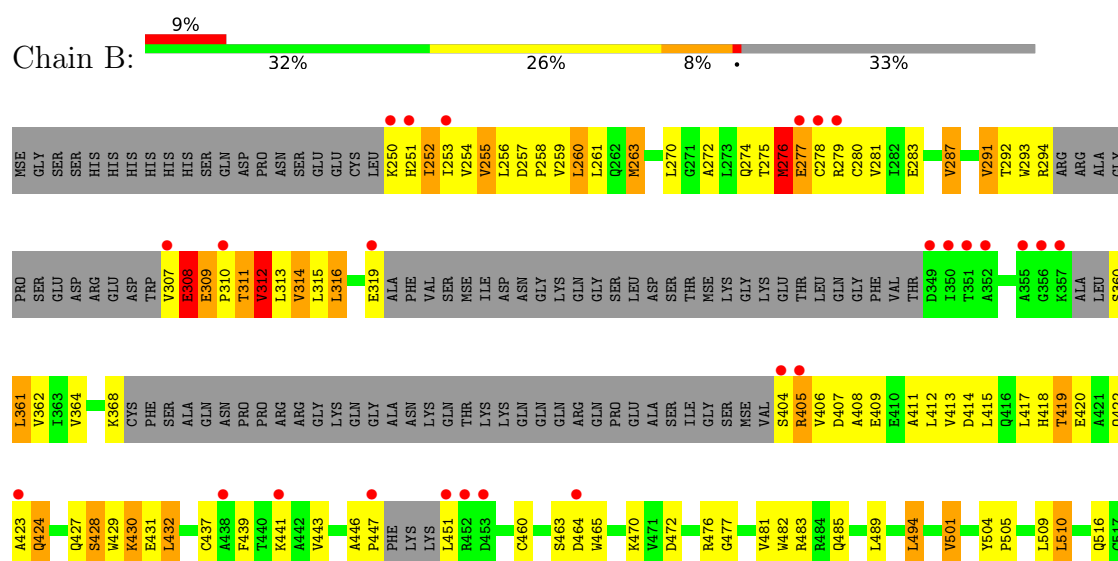
3 Residue-property plots

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: Mus81 protein



• Molecule 2: Crossover junction endonuclease EME1





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.96Å 88.96Å 169.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.56 – 2.80 37.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (37.56-2.80) 98.2 (37.56-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.04 (at 2.72Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.272 , 0.327 0.292 , 0.343	Depositor DCC
R_{free} test set	1863 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	3869	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 3.61% 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

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	0.64	5/2184 (0.2%)	1.07	14/2934 (0.5%)
2	B	0.63	3/1730 (0.2%)	1.06	9/2340 (0.4%)
All	All	0.64	8/3914 (0.2%)	1.06	23/5274 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	MSE	SE-CE	-9.07	1.68	1.95
1	A	396	MSE	SE-CE	-6.95	1.74	1.95
1	A	475	MSE	SE-CE	-6.17	1.76	1.95
2	B	557	MSE	SE-CE	-5.74	1.78	1.95
2	B	276	MSE	SE-CE	-5.71	1.78	1.95
1	A	515	MSE	SE-CE	-5.69	1.78	1.95
2	B	263	MSE	SE-CE	-5.39	1.79	1.95
1	A	541	MSE	CG-SE	-5.12	1.80	1.95

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	TYR	N-CA-C	-9.82	103.43	114.62
2	B	309	GLU	N-CA-C	8.86	127.41	109.60
1	A	328	CYS	N-CA-C	-8.82	100.64	111.40
2	B	422	GLN	N-CA-C	-8.29	99.36	110.55
1	A	588	LYS	N-CA-C	-7.04	101.24	110.33
1	A	408	PHE	N-CA-C	6.97	118.57	110.97
1	A	444	LEU	N-CA-C	-6.81	103.78	111.07
1	A	315	SER	CA-C-N	6.78	128.31	119.84
1	A	315	SER	C-N-CA	6.78	128.31	119.84
2	B	504	TYR	CA-C-N	6.57	128.05	119.84
2	B	504	TYR	C-N-CA	6.57	128.05	119.84
1	A	577	LYS	N-CA-C	-6.39	104.23	111.07
1	A	589	LEU	N-CA-C	-6.38	98.30	109.02
1	A	313	HIS	N-CA-C	6.25	121.04	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	362	VAL	N-CA-C	6.20	117.08	108.89
2	B	430	LYS	N-CA-C	-6.13	104.51	111.07
1	A	578	GLU	N-CA-C	-5.86	98.31	110.80
1	A	586	TYR	N-CA-C	5.77	117.95	109.24
1	A	481	LYS	N-CA-C	-5.68	101.43	109.96
2	B	407	ASP	N-CA-C	-5.07	105.88	111.71
1	A	367	ARG	N-CA-C	5.06	117.55	109.96
2	B	550	SER	N-CA-C	-5.05	106.29	112.90
2	B	312	VAL	N-CA-C	5.03	119.79	109.34

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	2155	0	2198	149	0
2	B	1714	0	1663	119	0
All	All	3869	0	3861	258	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 33.

All (258) 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:312:TRP:HE1	1:A:314:LEU:HB2	1.05	1.13
1:A:316:PRO:HD3	1:A:487:THR:HA	1.30	1.08
2:B:566:LEU:HD12	2:B:566:LEU:H	1.13	1.06
1:A:487:THR:HG23	1:A:488:LEU:H	1.28	0.99
2:B:555:LEU:HD21	2:B:564:LEU:HD21	1.45	0.97
2:B:294:ARG:HA	2:B:309:GLU:HA	1.47	0.95
1:A:412:LYS:NZ	1:A:451:THR:HG22	1.82	0.95
1:A:358:ASN:H	1:A:521:ASN:HD21	1.19	0.91
1:A:312:TRP:NE1	1:A:314:LEU:HB2	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:THR:HG22	1:A:372:PRO:HD2	1.55	0.88
1:A:412:LYS:HZ3	1:A:451:THR:HG22	1.41	0.85
1:A:487:THR:O	1:A:488:LEU:HB2	1.77	0.84
1:A:522:TYR:O	1:A:525:ILE:HG22	1.78	0.84
1:A:600:THR:HA	1:A:603:GLN:HE21	1.43	0.84
2:B:256:LEU:HD22	2:B:261:LEU:HD21	1.59	0.83
1:A:447:ALA:O	1:A:451:THR:HG23	1.78	0.83
2:B:272:ALA:O	2:B:275:THR:HG22	1.80	0.82
1:A:358:ASN:HB2	1:A:521:ASN:ND2	1.94	0.81
2:B:545:ILE:HG23	2:B:549:LEU:HD12	1.62	0.81
2:B:257:ASP:OD2	2:B:259:VAL:HG12	1.81	0.80
2:B:263:MSE:HE1	2:B:316:LEU:HD22	1.65	0.78
1:A:376:GLN:OE1	1:A:380:PRO:HD3	1.85	0.77
1:A:326:ASP:CG	1:A:327:LEU:H	1.92	0.77
1:A:522:TYR:CZ	1:A:526:LYS:HD2	2.20	0.77
1:A:329:GLU:O	1:A:330:THR:HB	1.83	0.77
1:A:591:ARG:H	1:A:591:ARG:HD3	1.49	0.77
1:A:475:MSE:SE	2:B:413:VAL:HG13	2.35	0.76
2:B:566:LEU:H	2:B:566:LEU:CD1	1.93	0.76
2:B:544:ARG:O	2:B:545:ILE:HB	1.86	0.74
2:B:292:THR:HG22	2:B:313:LEU:HG	1.68	0.74
2:B:544:ARG:HD2	2:B:544:ARG:N	2.04	0.73
2:B:316:LEU:HD11	2:B:432:LEU:HD11	1.71	0.73
2:B:307:VAL:HG23	2:B:308:GLU:H	1.53	0.73
1:A:481:LYS:O	1:A:482:LEU:HB2	1.88	0.72
2:B:316:LEU:HD21	2:B:432:LEU:HD11	1.72	0.70
1:A:316:PRO:CD	1:A:487:THR:HA	2.17	0.70
2:B:368:LYS:CB	2:B:427:GLN:HB3	2.22	0.69
1:A:312:TRP:CD1	1:A:312:TRP:C	2.70	0.69
1:A:320:ASP:O	1:A:366:ALA:HA	1.94	0.68
1:A:599:ARG:HG3	1:A:599:ARG:HH11	1.59	0.68
2:B:277:GLU:OE2	2:B:278:CYS:N	2.27	0.67
2:B:312:VAL:O	2:B:313:LEU:HD12	1.95	0.67
2:B:556:GLN:HB3	2:B:566:LEU:HD21	1.76	0.67
1:A:535:VAL:O	1:A:539:GLN:HG3	1.94	0.67
2:B:404:SER:C	2:B:406:VAL:H	2.03	0.66
2:B:409:GLU:O	2:B:413:VAL:HG23	1.94	0.66
2:B:439:PHE:O	2:B:443:VAL:HG23	1.94	0.66
2:B:566:LEU:HD12	2:B:566:LEU:N	1.98	0.65
2:B:441:LYS:NZ	2:B:441:LYS:HB3	2.11	0.65
1:A:426:LEU:HD21	1:A:468:SER:OG	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TYR:HA	1:A:486:CYS:HB2	1.78	0.65
1:A:522:TYR:CE2	1:A:526:LYS:HD2	2.31	0.65
1:A:550:LYS:O	1:A:554:VAL:HG12	1.96	0.65
1:A:482:LEU:HD13	1:A:510:LEU:HD11	1.77	0.65
2:B:555:LEU:HD21	2:B:564:LEU:CD2	2.23	0.64
1:A:487:THR:HG23	1:A:488:LEU:N	2.09	0.64
1:A:531:THR:OG1	1:A:534:GLU:HG3	1.98	0.64
2:B:551:ARG:O	2:B:555:LEU:HB2	1.98	0.64
2:B:428:SER:O	2:B:429:TRP:HB2	1.98	0.64
2:B:253:ILE:HA	2:B:279:ARG:HB3	1.80	0.63
1:A:588:LYS:O	1:A:589:LEU:HB2	1.99	0.62
2:B:489:LEU:CD1	2:B:553:ILE:HG12	2.28	0.62
2:B:549:LEU:HD13	2:B:549:LEU:O	2.00	0.62
1:A:389:TYR:HE1	1:A:422:LYS:HG3	1.63	0.62
1:A:578:GLU:O	1:A:580:LEU:N	2.32	0.62
1:A:539:GLN:HE22	2:B:556:GLN:HE22	1.47	0.61
2:B:312:VAL:C	2:B:313:LEU:HD12	2.25	0.61
1:A:481:LYS:O	1:A:482:LEU:CB	2.47	0.61
2:B:549:LEU:HD23	2:B:552:ARG:NH2	2.15	0.61
1:A:514:LEU:N	1:A:514:LEU:HD23	2.17	0.60
1:A:329:GLU:O	1:A:330:THR:CB	2.48	0.60
2:B:483:ARG:HA	2:B:501:VAL:HG21	1.83	0.60
2:B:294:ARG:HA	2:B:309:GLU:CA	2.27	0.60
1:A:482:LEU:HD13	1:A:510:LEU:CD1	2.31	0.59
1:A:389:TYR:HD1	1:A:422:LYS:HB2	1.67	0.59
2:B:311:THR:HB	2:B:360:SER:O	2.03	0.59
1:A:389:TYR:CE1	1:A:422:LYS:HG3	2.37	0.59
2:B:307:VAL:HG23	2:B:308:GLU:N	2.18	0.58
1:A:599:ARG:HG3	1:A:599:ARG:NH1	2.19	0.58
1:A:439:ILE:HD12	1:A:439:ILE:N	2.19	0.58
2:B:419:THR:HG22	2:B:420:GLU:H	1.69	0.58
1:A:412:LYS:HZ2	1:A:451:THR:HG22	1.68	0.57
1:A:478:TYR:O	1:A:481:LYS:O	2.21	0.57
2:B:252:ILE:HG22	2:B:307:VAL:HA	1.87	0.57
2:B:544:ARG:HG2	2:B:544:ARG:HH11	1.69	0.57
1:A:487:THR:CG2	1:A:488:LEU:H	2.10	0.57
1:A:591:ARG:HH21	1:A:591:ARG:HG3	1.70	0.57
1:A:538:ARG:HD3	2:B:460:CYS:HB2	1.87	0.57
2:B:294:ARG:C	2:B:307:VAL:O	2.47	0.57
1:A:526:LYS:NZ	1:A:526:LYS:HB3	2.20	0.57
1:A:371:THR:CG2	1:A:372:PRO:HD2	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ARG:O	1:A:603:GLN:HG3	2.05	0.56
2:B:404:SER:O	2:B:406:VAL:N	2.38	0.56
2:B:276:MSE:HE3	2:B:278:CYS:SG	2.45	0.56
2:B:441:LYS:HB3	2:B:441:LYS:HZ3	1.70	0.56
1:A:340:GLU:O	1:A:342:VAL:N	2.38	0.56
1:A:319:TYR:OH	1:A:483:TYR:O	2.23	0.56
2:B:293:TRP:C	2:B:310:PRO:HD2	2.30	0.56
2:B:311:THR:C	2:B:312:VAL:HG23	2.30	0.56
1:A:578:GLU:C	1:A:580:LEU:H	2.13	0.56
1:A:324:CYS:O	1:A:362:PHE:HA	2.06	0.55
1:A:326:ASP:CG	1:A:327:LEU:N	2.61	0.55
2:B:551:ARG:HB3	2:B:551:ARG:NH1	2.20	0.55
1:A:389:TYR:CD1	1:A:422:LYS:HB2	2.41	0.55
1:A:358:ASN:N	1:A:521:ASN:HD21	1.97	0.55
2:B:408:ALA:O	2:B:412:LEU:HG	2.07	0.55
2:B:405:ARG:O	2:B:408:ALA:HB3	2.07	0.55
2:B:311:THR:OG1	2:B:312:VAL:N	2.40	0.54
1:A:591:ARG:HG3	1:A:591:ARG:NH2	2.22	0.54
1:A:412:LYS:O	1:A:416:LYS:HG3	2.07	0.54
1:A:324:CYS:HB2	1:A:363:LEU:CD2	2.37	0.54
2:B:532:VAL:O	2:B:533:ARG:HB2	2.07	0.54
1:A:315:SER:CB	1:A:316:PRO:HD2	2.38	0.54
2:B:256:LEU:HD23	2:B:260:LEU:CD2	2.37	0.54
2:B:309:GLU:HG3	2:B:310:PRO:O	2.08	0.53
1:A:314:LEU:HD21	1:A:319:TYR:HB3	1.91	0.53
2:B:546:GLY:O	2:B:550:SER:HB2	2.08	0.53
1:A:408:PHE:CZ	1:A:412:LYS:HE2	2.43	0.53
2:B:494:LEU:HD13	2:B:494:LEU:C	2.34	0.53
2:B:472:ASP:OD2	2:B:476:ARG:HB2	2.09	0.52
2:B:258:PRO:HD3	2:B:283:GLU:O	2.09	0.52
2:B:275:THR:HG23	2:B:276:MSE:N	2.25	0.52
1:A:326:ASP:OD2	1:A:327:LEU:N	2.37	0.52
1:A:429:GLU:O	1:A:430:CYS:HB2	2.10	0.52
1:A:363:LEU:C	1:A:363:LEU:HD23	2.36	0.51
1:A:368:GLU:OE2	1:A:383:LYS:HG3	2.11	0.51
1:A:526:LYS:HB3	1:A:526:LYS:HZ3	1.76	0.51
2:B:250:LYS:NZ	2:B:276:MSE:SE	2.93	0.51
2:B:293:TRP:O	2:B:310:PRO:HD2	2.10	0.51
2:B:411:ALA:O	2:B:415:LEU:N	2.44	0.51
1:A:340:GLU:O	1:A:343:LYS:HG2	2.10	0.51
1:A:325:VAL:HG12	1:A:326:ASP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:SER:O	1:A:573:SER:CB	2.58	0.51
2:B:257:ASP:O	2:B:260:LEU:HB3	2.11	0.51
1:A:462:VAL:HG13	1:A:467:GLU:HB3	1.93	0.50
1:A:408:PHE:CE2	1:A:412:LYS:HE2	2.47	0.50
1:A:324:CYS:HB2	1:A:363:LEU:HD23	1.94	0.50
1:A:416:LYS:HG2	1:A:457:PHE:HE1	1.76	0.50
2:B:489:LEU:HD21	2:B:556:GLN:HG2	1.94	0.50
1:A:319:TYR:CD1	1:A:319:TYR:C	2.90	0.49
1:A:358:ASN:HB2	1:A:521:ASN:HD21	1.70	0.49
1:A:477:ARG:HG3	1:A:477:ARG:HH11	1.76	0.49
1:A:391:ILE:CG2	1:A:392:GLU:N	2.74	0.49
2:B:316:LEU:HD21	2:B:432:LEU:CD1	2.40	0.49
1:A:577:LYS:C	1:A:578:GLU:O	2.45	0.49
1:A:340:GLU:O	1:A:341:LEU:C	2.55	0.49
1:A:607:THR:O	1:A:608:ARG:HB2	2.12	0.49
2:B:437:CYS:O	2:B:441:LYS:HG3	2.11	0.49
1:A:353:ASP:OD2	1:A:355:ARG:NE	2.38	0.49
2:B:252:ILE:HD12	2:B:252:ILE:O	2.12	0.49
1:A:341:LEU:O	1:A:345:LEU:HB2	2.12	0.49
1:A:543:ILE:HB	1:A:546:VAL:CG1	2.43	0.49
2:B:312:VAL:O	2:B:313:LEU:CD1	2.61	0.49
1:A:340:GLU:HA	1:A:343:LYS:NZ	2.27	0.48
1:A:390:ILE:HB	1:A:420:LEU:HD23	1.95	0.48
1:A:312:TRP:CH2	1:A:385:LEU:HD11	2.48	0.48
1:A:314:LEU:HD23	1:A:314:LEU:C	2.39	0.48
1:A:357:LEU:HD21	1:A:363:LEU:HD22	1.95	0.48
1:A:483:TYR:O	1:A:485:ASN:N	2.46	0.48
2:B:532:VAL:O	2:B:533:ARG:CB	2.61	0.48
1:A:397:ASP:O	1:A:400:CYS:HB2	2.13	0.48
1:A:449:VAL:HG11	2:B:439:PHE:HA	1.96	0.48
2:B:291:VAL:CG1	2:B:314:VAL:HB	2.44	0.48
1:A:557:HIS:CD2	1:A:584:VAL:HG22	2.48	0.48
2:B:544:ARG:O	2:B:545:ILE:CB	2.58	0.48
1:A:312:TRP:HE1	1:A:314:LEU:CB	1.98	0.47
1:A:568:TYR:HE1	1:A:577:LYS:O	1.96	0.47
2:B:428:SER:C	2:B:430:LYS:H	2.22	0.47
1:A:313:HIS:ND1	1:A:314:LEU:N	2.62	0.47
2:B:252:ILE:HG22	2:B:307:VAL:O	2.14	0.47
1:A:313:HIS:CE1	1:A:315:SER:OG	2.68	0.47
1:A:513:SER:C	1:A:514:LEU:HD23	2.38	0.47
1:A:313:HIS:HE1	1:A:315:SER:OG	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:SER:C	2:B:406:VAL:N	2.70	0.47
1:A:329:GLU:O	1:A:339:GLN:HG2	2.14	0.47
2:B:275:THR:CG2	2:B:276:MSE:N	2.78	0.47
1:A:391:ILE:HG22	1:A:392:GLU:N	2.31	0.46
2:B:430:LYS:HD2	2:B:430:LYS:HA	1.75	0.46
1:A:346:GLN:O	1:A:349:SER:N	2.38	0.46
2:B:287:VAL:CG2	2:B:315:LEU:HD11	2.47	0.45
1:A:395:ARG:O	1:A:396:MSE:C	2.60	0.45
1:A:538:ARG:CD	2:B:460:CYS:HB2	2.46	0.45
2:B:316:LEU:CD1	2:B:432:LEU:HD11	2.45	0.45
2:B:250:LYS:HZ3	2:B:276:MSE:SE	2.50	0.45
2:B:482:TRP:CD1	2:B:501:VAL:HG22	2.52	0.45
1:A:344:GLU:CD	1:A:466:LYS:HE3	2.41	0.44
2:B:420:GLU:OE2	2:B:420:GLU:N	2.50	0.44
2:B:549:LEU:O	2:B:549:LEU:HD22	2.18	0.44
1:A:326:ASP:HB2	1:A:357:LEU:HD12	2.00	0.44
2:B:364:VAL:O	2:B:423:ALA:HA	2.17	0.44
1:A:361:ASP:O	1:A:391:ILE:O	2.35	0.44
1:A:484:GLN:HE21	1:A:484:GLN:HA	1.82	0.44
2:B:419:THR:HG22	2:B:420:GLU:N	2.32	0.44
2:B:451:LEU:N	2:B:451:LEU:HD12	2.33	0.44
1:A:529:CYS:SG	2:B:565:SER:HB3	2.57	0.44
1:A:608:ARG:O	2:B:509:LEU:HG	2.18	0.44
2:B:544:ARG:HG2	2:B:544:ARG:NH1	2.33	0.44
1:A:481:LYS:HE2	1:A:481:LYS:HB3	1.80	0.44
2:B:530:ILE:HB	2:B:545:ILE:HD12	2.00	0.43
1:A:358:ASN:CB	1:A:521:ASN:HD21	2.32	0.43
2:B:521:LYS:HZ2	2:B:521:LYS:C	2.27	0.43
1:A:429:GLU:O	1:A:430:CYS:CB	2.67	0.43
2:B:481:VAL:O	2:B:485:GLN:HG3	2.19	0.43
1:A:314:LEU:CD2	1:A:319:TYR:HB3	2.49	0.43
1:A:396:MSE:HE3	1:A:430:CYS:HA	2.01	0.43
2:B:560:LEU:N	2:B:560:LEU:HD22	2.33	0.43
1:A:591:ARG:H	1:A:591:ARG:CD	2.24	0.43
1:A:354:VAL:O	1:A:354:VAL:HG12	2.19	0.43
1:A:483:TYR:CD2	1:A:488:LEU:HD11	2.54	0.43
2:B:319:GLU:O	2:B:319:GLU:CG	2.67	0.43
1:A:357:LEU:HD22	1:A:363:LEU:HD13	2.01	0.43
2:B:250:LYS:C	2:B:251:HIS:ND1	2.76	0.43
2:B:360:SER:O	2:B:361:LEU:CB	2.67	0.43
1:A:464:ASP:CG	1:A:465:ALA:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:ARG:HG2	2:B:566:LEU:HB3	2.01	0.42
2:B:254:VAL:HG13	2:B:254:VAL:O	2.19	0.42
2:B:255:VAL:HA	2:B:281:VAL:O	2.18	0.42
2:B:551:ARG:NH1	2:B:567:ASP:O	2.53	0.42
1:A:483:TYR:O	1:A:484:GLN:C	2.62	0.42
1:A:568:TYR:O	1:A:577:LYS:NZ	2.51	0.42
1:A:323:LEU:HD12	1:A:324:CYS:H	1.84	0.42
2:B:414:ASP:O	2:B:418:HIS:HD2	2.02	0.42
1:A:612:SER:C	2:B:477:GLY:H	2.28	0.42
1:A:330:THR:O	1:A:330:THR:HG22	2.20	0.42
1:A:390:ILE:O	1:A:390:ILE:HG23	2.20	0.42
2:B:250:LYS:O	2:B:250:LYS:HG3	2.20	0.42
1:A:365:VAL:CG2	1:A:384:GLU:HB3	2.50	0.42
1:A:404:ILE:CG1	1:A:439:ILE:HD11	2.50	0.42
2:B:428:SER:OG	2:B:431:GLU:HG3	2.20	0.42
2:B:424:GLN:HE21	2:B:424:GLN:HB2	1.54	0.41
1:A:344:GLU:OE1	1:A:466:LYS:HE3	2.20	0.41
2:B:464:ASP:OD1	2:B:465:TRP:N	2.51	0.41
1:A:451:THR:HA	1:A:455:ASP:OD2	2.21	0.41
1:A:595:PRO:HG2	1:A:596:ALA:H	1.85	0.41
1:A:611:LEU:HD12	2:B:482:TRP:HB2	2.03	0.41
1:A:612:SER:OXT	2:B:477:GLY:N	2.46	0.41
2:B:547:PRO:HG2	2:B:548:GLU:H	1.84	0.41
1:A:326:ASP:OD1	1:A:357:LEU:N	2.43	0.41
2:B:441:LYS:NZ	2:B:441:LYS:CB	2.80	0.41
1:A:359:VAL:O	1:A:359:VAL:HG13	2.20	0.41
1:A:585:LYS:HD2	1:A:590:LYS:O	2.20	0.41
1:A:325:VAL:O	1:A:354:VAL:HA	2.21	0.41
1:A:361:ASP:O	1:A:362:PHE:HB2	2.21	0.41
1:A:543:ILE:O	1:A:546:VAL:CG1	2.69	0.41
2:B:270:LEU:HG	2:B:274:GLN:NE2	2.36	0.41
2:B:294:ARG:C	2:B:308:GLU:O	2.64	0.41
1:A:404:ILE:HG13	1:A:439:ILE:HD11	2.02	0.41
1:A:412:LYS:NZ	1:A:455:ASP:OD2	2.52	0.41
1:A:460:LYS:HD2	1:A:460:LYS:HA	1.89	0.41
1:A:312:TRP:CD1	1:A:313:HIS:N	2.89	0.40
1:A:462:VAL:CG1	1:A:463:GLN:N	2.83	0.40
1:A:589:LEU:O	1:A:590:LYS:HB3	2.21	0.40
1:A:599:ARG:O	1:A:600:THR:C	2.63	0.40
2:B:294:ARG:C	2:B:308:GLU:C	2.89	0.40
2:B:510:LEU:O	2:B:510:LEU:HD22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:VAL:HG12	2:B:417:LEU:HD12	2.02	0.40
2:B:446:ALA:HA	2:B:447:PRO:HA	1.89	0.40
2:B:527:LEU:HB3	2:B:530:ILE:HD12	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	263/311 (85%)	218 (83%)	31 (12%)	14 (5%)	1	5
2	B	214/341 (63%)	179 (84%)	23 (11%)	12 (6%)	1	4
All	All	477/652 (73%)	397 (83%)	54 (11%)	26 (6%)	1	4

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	PRO
1	A	341	LEU
1	A	482	LEU
1	A	484	GLN
1	A	488	LEU
2	B	308	GLU
2	B	312	VAL
2	B	361	LEU
2	B	405	ARG
2	B	533	ARG
1	A	439	ILE
1	A	487	THR
1	A	573	SER
1	A	590	LYS
2	B	276	MSE

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Mol	Chain	Res	Type
2	B	428	SER
2	B	545	ILE
1	A	388	ASP
1	A	579	LYS
1	A	429	GLU
2	B	311	THR
1	A	587	GLY
2	B	277	GLU
2	B	280	CYS
2	B	505	PRO
1	A	317	GLY

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	241/264 (91%)	212 (88%)	29 (12%)	5	17
2	B	173/282 (61%)	153 (88%)	20 (12%)	5	18
All	All	414/546 (76%)	365 (88%)	49 (12%)	5	17

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	TRP
1	A	315	SER
1	A	328	CYS
1	A	339	GLN
1	A	341	LEU
1	A	361	ASP
1	A	363	LEU
1	A	371	THR
1	A	386	VAL
1	A	407	ARG
1	A	412	LYS
1	A	420	LEU

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Mol	Chain	Res	Type
1	A	421	ARG
1	A	439	ILE
1	A	462	VAL
1	A	463	GLN
1	A	466	LYS
1	A	468	SER
1	A	484	GLN
1	A	485	ASN
1	A	509	ASN
1	A	514	LEU
1	A	521	ASN
1	A	546	VAL
1	A	554	VAL
1	A	555	LEU
1	A	561	VAL
1	A	590	LYS
1	A	591	ARG
2	B	252	ILE
2	B	255	VAL
2	B	260	LEU
2	B	287	VAL
2	B	291	VAL
2	B	308	GLU
2	B	312	VAL
2	B	314	VAL
2	B	316	LEU
2	B	419	THR
2	B	424	GLN
2	B	432	LEU
2	B	463	SER
2	B	470	LYS
2	B	494	LEU
2	B	501	VAL
2	B	510	LEU
2	B	516	GLN
2	B	555	LEU
2	B	566	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	HIS

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Mol	Chain	Res	Type
1	A	348	ASN
1	A	358	ASN
1	A	445	GLN
1	A	446	GLN
1	A	450	ASN
1	A	452	GLN
1	A	480	GLN
1	A	484	GLN
1	A	485	ASN
1	A	521	ASN
1	A	557	HIS
1	A	603	GLN
2	B	274	GLN
2	B	416	GLN
2	B	418	HIS
2	B	424	GLN
2	B	427	GLN
2	B	524	GLN
2	B	556	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 ⓘ

There are no ligands in this entry.

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

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	267/311 (85%)	0.66	17 (6%) 25 18	21, 47, 68, 85	0
2	B	224/341 (65%)	0.83	30 (13%) 7 5	20, 48, 79, 86	0
All	All	491/652 (75%)	0.73	47 (9%) 13 10	20, 48, 72, 86	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	349	ASP	6.0
1	A	329	GLU	5.7
1	A	508	ALA	4.6
2	B	352	ALA	3.5
2	B	404	SER	3.3
2	B	423	ALA	3.3
2	B	438	ALA	3.3
2	B	319	GLU	3.2
2	B	278	CYS	3.1
2	B	464	ASP	3.1
2	B	279	ARG	3.1
2	B	357	LYS	3.1
2	B	250	LYS	3.0
1	A	327	LEU	3.0
2	B	356	GLY	3.0
2	B	518	PHE	2.9
1	A	317	GLY	2.9
2	B	277	GLU	2.7
2	B	451	LEU	2.7
2	B	567	ASP	2.7
1	A	340	GLU	2.7
1	A	431	GLY	2.6
2	B	533	ARG	2.6
1	A	575	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	355	ALA	2.6
2	B	453	ASP	2.4
1	A	339	GLN	2.4
2	B	350	ILE	2.4
2	B	307	VAL	2.4
1	A	464	ASP	2.3
1	A	397	ASP	2.3
2	B	441	LYS	2.3
2	B	251	HIS	2.3
2	B	405	ARG	2.3
1	A	389	TYR	2.3
1	A	510	LEU	2.2
2	B	549	LEU	2.2
1	A	590	LYS	2.2
2	B	253	ILE	2.2
2	B	447	PRO	2.2
2	B	452	ARG	2.2
2	B	351	THR	2.2
1	A	312	TRP	2.1
2	B	310	PRO	2.1
1	A	330	THR	2.1
1	A	328	CYS	2.0
1	A	519	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.