



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:46 AM UTC

PDB ID : 2ZIU / pdb_00002ziu
Title : Crystal structure of the Mus81-Eme1 complex
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Deposited on : 2008-02-25
Resolution : 2.70 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

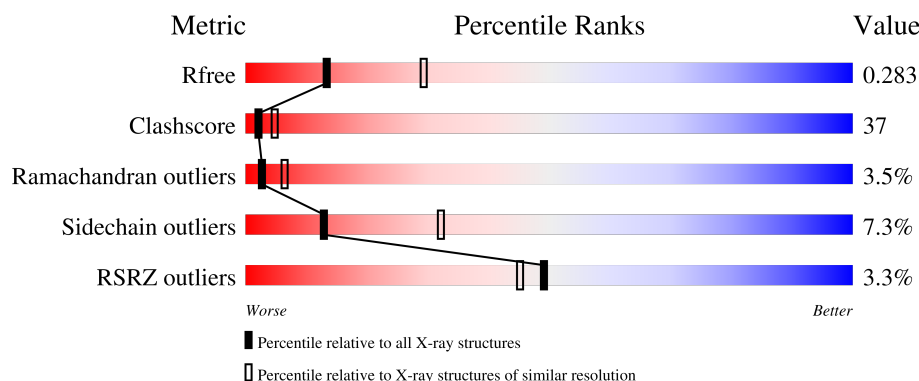
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	
2	B	341	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4296 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	281	Total	C	N	O	S	0	0	0
			2227	1409	392	411	15			

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2013	1266	353	382	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	230	MET	-	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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Chain	Residue	Modelled	Actual	Comment	Reference
B	245	SER	-	expression tag	UNP Q96AY2

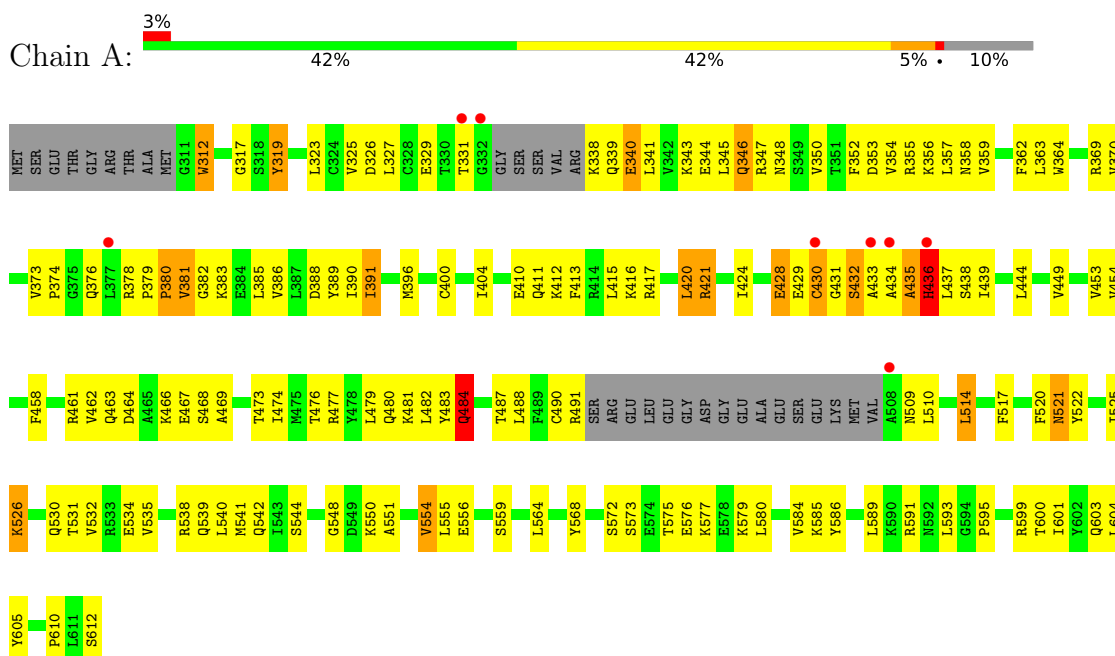
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	30	Total O 30 30	0	0
3	B	26	Total O 26 26	0	0

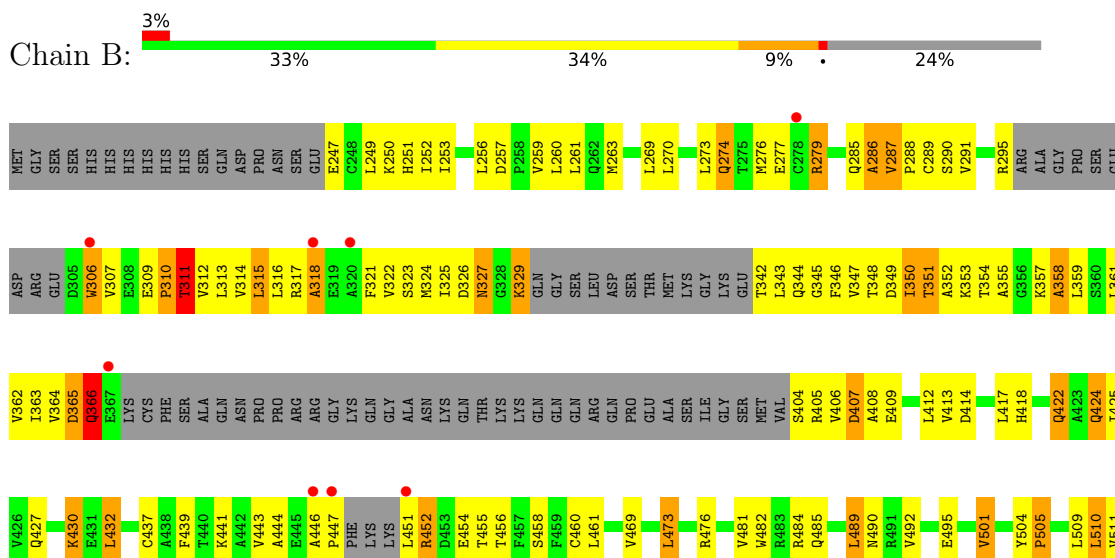
3 Residue-property plots

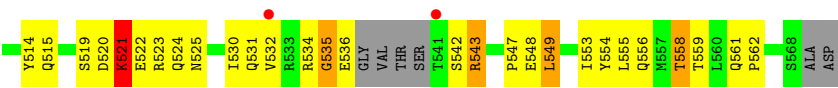
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	88.68Å 88.68Å 170.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.03 – 2.70 29.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.03-2.70) 97.3 (29.03-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.286 0.233 , 0.283	Depositor DCC
R_{free} test set	1026 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4296	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.47	0/2262	0.99	13/3045 (0.4%)
2	B	0.49	0/2038	1.04	14/2758 (0.5%)
All	All	0.48	0/4300	1.02	27/5803 (0.5%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	VAL	N-CA-C	7.59	117.66	110.53
2	B	345	GLY	N-CA-C	-7.03	103.95	113.37
2	B	532	VAL	N-CA-C	6.71	118.27	110.62
2	B	535	GLY	N-CA-C	-6.58	106.09	113.79
1	A	444	LEU	N-CA-C	-6.19	104.22	110.97
1	A	454	VAL	N-CA-C	5.83	116.48	110.82
2	B	365	ASP	N-CA-C	5.78	123.11	110.80
1	A	564	LEU	N-CA-C	-5.73	105.04	111.28
2	B	504	TYR	CA-C-N	5.72	127.00	119.84
2	B	504	TYR	C-N-CA	5.72	127.00	119.84
1	A	421	ARG	N-CA-C	5.72	119.73	112.87
1	A	468	SER	N-CA-C	-5.71	105.14	111.36
2	B	558	THR	N-CA-C	5.58	120.96	114.04
2	B	350	ILE	N-CA-C	-5.55	104.91	110.30
1	A	379	PRO	CA-C-N	5.46	126.67	119.84
1	A	379	PRO	C-N-CA	5.46	126.67	119.84
1	A	391	ILE	N-CA-C	5.34	116.16	108.48
1	A	382	GLY	N-CA-C	5.30	120.13	112.82
2	B	521	LYS	N-CA-C	-5.26	106.36	112.89
2	B	561	GLN	CA-C-N	5.26	124.93	119.56
2	B	561	GLN	C-N-CA	5.26	124.93	119.56
2	B	366	GLN	N-CA-C	-5.25	99.62	110.80
2	B	252	ILE	N-CA-C	5.24	116.13	108.53
2	B	407	ASP	N-CA-C	-5.18	105.07	111.33
1	A	346	GLN	N-CA-C	-5.08	106.94	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	556	GLU	N-CA-C	-5.04	105.98	111.82
1	A	386	VAL	N-CA-C	5.02	115.08	107.75

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	2227	0	2276	157	0
2	B	2013	0	2031	188	0
3	A	30	0	0	9	0
3	B	26	0	0	11	0
All	All	4296	0	4307	319	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 (319) 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:612:SER:OXT	2:B:476:ARG:HA	1.46	1.14
1:A:482:LEU:HD13	1:A:510:LEU:HD11	1.26	1.10
1:A:326:ASP:HB2	1:A:357:LEU:HD12	1.42	1.02
1:A:404:ILE:HG13	1:A:439:ILE:HD11	1.45	0.96
1:A:541:MET:HE1	2:B:461:LEU:HA	1.46	0.95
2:B:430:LYS:HA	2:B:430:LYS:HE3	1.48	0.93
2:B:365:ASP:CG	2:B:366:GLN:H	1.77	0.92
2:B:530:ILE:HA	2:B:534:ARG:HH12	1.34	0.91
1:A:396:MET:HG2	1:A:431:GLY:HA2	1.53	0.90
1:A:484:GLN:HE21	1:A:484:GLN:HA	1.37	0.89
3:A:11:HOH:O	2:B:455:THR:HG21	1.72	0.89
2:B:279:ARG:HH11	2:B:279:ARG:HB3	1.37	0.87
2:B:324:MET:HG3	2:B:343:LEU:HA	1.57	0.87
3:A:4:HOH:O	2:B:460:CYS:HB3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:VAL:HG13	1:A:467:GLU:HB3	1.60	0.83
2:B:530:ILE:HA	2:B:534:ARG:NH1	1.94	0.82
2:B:257:ASP:OD2	2:B:259:VAL:HG22	1.82	0.79
1:A:531:THR:OG1	1:A:534:GLU:HG3	1.83	0.78
2:B:455:THR:HG23	2:B:458:SER:H	1.48	0.78
2:B:279:ARG:HB3	2:B:279:ARG:NH1	1.99	0.76
2:B:247:GLU:HA	2:B:250:LYS:HE2	1.67	0.76
1:A:358:ASN:H	1:A:521:ASN:HD21	1.32	0.75
2:B:365:ASP:CG	2:B:366:GLN:N	2.46	0.74
1:A:350:VAL:HG21	1:A:473:THR:HG22	1.70	0.74
1:A:385:LEU:HD21	1:A:490:CYS:HB2	1.71	0.73
1:A:431:GLY:O	1:A:432:SER:HB2	1.89	0.72
1:A:438:SER:HB3	1:A:439:ILE:HD12	1.70	0.72
2:B:542:SER:O	2:B:543:ARG:HB2	1.90	0.71
2:B:249:LEU:HB2	2:B:277:GLU:HB2	1.72	0.71
2:B:351:THR:HA	2:B:354:THR:HB	1.71	0.71
1:A:329:GLU:HG2	1:A:362:PHE:CZ	2.27	0.70
2:B:306:TRP:HA	2:B:306:TRP:CE3	2.27	0.70
2:B:521:LYS:NZ	2:B:521:LYS:HB3	2.07	0.69
1:A:327:LEU:HD12	1:A:356:LYS:HD3	1.73	0.68
1:A:396:MET:HE3	1:A:430:CYS:HA	1.76	0.68
1:A:491:ARG:HD3	1:A:491:ARG:C	2.19	0.68
1:A:559:SER:HB2	2:B:562:PRO:HB3	1.76	0.68
1:A:432:SER:H	1:A:435:ALA:HB2	1.59	0.67
2:B:306:TRP:HA	2:B:306:TRP:HE3	1.58	0.67
1:A:348:ASN:OD1	1:A:473:THR:HG21	1.94	0.67
1:A:428:GLU:C	1:A:430:CYS:H	2.03	0.67
2:B:325:ILE:HG13	2:B:326:ASP:N	2.10	0.67
1:A:612:SER:C	3:A:17:HOH:O	2.39	0.66
2:B:260:LEU:HA	2:B:263:MET:HE2	1.77	0.66
1:A:542:GLN:HE21	2:B:484:ARG:HE	1.41	0.66
1:A:428:GLU:HG3	1:A:429:GLU:N	2.10	0.66
2:B:349:ASP:HA	2:B:352:ALA:HB3	1.77	0.66
2:B:313:LEU:HD11	2:B:362:VAL:CG2	2.26	0.66
2:B:424:GLN:HG3	2:B:425:ILE:N	2.09	0.66
2:B:324:MET:HG3	2:B:343:LEU:CA	2.27	0.65
1:A:522:TYR:O	1:A:525:ILE:HG22	1.96	0.65
1:A:338:LYS:HE2	3:A:15:HOH:O	1.95	0.65
1:A:466:LYS:O	1:A:469:ALA:HB3	1.97	0.64
2:B:543:ARG:HG3	3:B:34:HOH:O	1.97	0.64
2:B:313:LEU:HD11	2:B:362:VAL:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:VAL:HG23	3:B:23:HOH:O	1.97	0.63
2:B:439:PHE:O	2:B:443:VAL:HG23	1.99	0.63
1:A:327:LEU:HG	1:A:355:ARG:O	1.98	0.63
2:B:519:SER:O	2:B:522:GLU:HB3	1.99	0.63
1:A:573:SER:HB3	1:A:576:GLU:HB2	1.79	0.63
2:B:309:GLU:HG3	2:B:310:PRO:HD2	1.81	0.63
1:A:550:LYS:O	1:A:554:VAL:HG12	1.99	0.62
2:B:357:LYS:O	2:B:358:ALA:HB3	1.98	0.62
2:B:404:SER:OG	2:B:406:VAL:HG22	1.98	0.62
1:A:526:LYS:NZ	1:A:526:LYS:HB3	2.14	0.62
1:A:612:SER:OXT	2:B:476:ARG:CA	2.36	0.62
1:A:417:ARG:NH2	2:B:456:THR:HG23	2.14	0.62
1:A:491:ARG:HD3	1:A:491:ARG:O	1.99	0.62
2:B:315:LEU:HD21	2:B:432:LEU:HD11	1.82	0.61
1:A:551:ALA:O	1:A:555:LEU:HD13	2.00	0.61
2:B:354:THR:HG23	2:B:357:LYS:HB2	1.82	0.61
2:B:531:GLN:H	2:B:534:ARG:NH1	1.99	0.60
2:B:256:LEU:HD22	2:B:261:LEU:HD21	1.82	0.60
1:A:317:GLY:O	1:A:369:ARG:NH1	2.35	0.60
1:A:380:PRO:O	1:A:381:VAL:HB	2.01	0.60
1:A:430:CYS:SG	1:A:463:GLN:HG3	2.42	0.59
1:A:439:ILE:HD12	1:A:439:ILE:N	2.17	0.59
2:B:350:ILE:HG21	2:B:359:LEU:HD22	1.84	0.59
2:B:354:THR:O	2:B:355:ALA:HB3	2.03	0.59
1:A:354:VAL:O	1:A:354:VAL:HG12	2.02	0.59
2:B:348:THR:O	2:B:352:ALA:N	2.36	0.59
1:A:482:LEU:HD13	1:A:510:LEU:CD1	2.17	0.58
2:B:327:ASN:ND2	2:B:342:THR:O	2.35	0.58
2:B:295:ARG:HG3	2:B:307:VAL:HG13	1.85	0.58
2:B:344:GLN:HA	3:B:23:HOH:O	2.03	0.58
2:B:531:GLN:H	2:B:534:ARG:CZ	2.17	0.58
1:A:388:ASP:OD2	1:A:421:ARG:NH2	2.37	0.58
1:A:477:ARG:O	1:A:481:LYS:HG2	2.04	0.58
2:B:346:PHE:O	2:B:350:ILE:HG13	2.04	0.58
1:A:541:MET:HE2	1:A:548:GLY:HA2	1.85	0.58
1:A:463:GLN:O	1:A:463:GLN:HG2	2.04	0.58
1:A:344:GLU:HG3	1:A:466:LYS:HG3	1.86	0.57
2:B:247:GLU:CA	2:B:250:LYS:HE2	2.32	0.57
2:B:523:ARG:NH2	3:B:16:HOH:O	2.36	0.57
2:B:354:THR:CG2	2:B:357:LYS:H	2.17	0.57
2:B:405:ARG:O	2:B:409:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:511:VAL:O	2:B:515:GLN:HG2	2.05	0.57
2:B:555:LEU:O	2:B:559:THR:HG22	2.03	0.57
2:B:312:VAL:HG21	2:B:357:LYS:HD2	1.86	0.57
2:B:253:ILE:HG13	2:B:279:ARG:NH1	2.19	0.57
2:B:247:GLU:HA	2:B:250:LYS:CE	2.35	0.57
2:B:312:VAL:CG2	2:B:357:LYS:HD2	2.35	0.57
2:B:554:TYR:O	2:B:558:THR:HB	2.05	0.57
1:A:550:LYS:HB3	1:A:593:LEU:HD21	1.87	0.56
2:B:365:ASP:C	2:B:366:GLN:HG2	2.30	0.56
2:B:520:ASP:HA	2:B:523:ARG:HH11	1.70	0.56
1:A:542:GLN:NE2	2:B:484:ARG:HE	2.04	0.56
1:A:331:THR:HA	1:A:338:LYS:HE3	1.86	0.56
2:B:324:MET:HA	2:B:327:ASN:HD22	1.69	0.56
1:A:462:VAL:CG1	1:A:467:GLU:HB3	2.34	0.56
1:A:326:ASP:CB	1:A:357:LEU:HD12	2.29	0.56
2:B:310:PRO:HB2	2:B:357:LYS:O	2.06	0.56
1:A:339:GLN:HG3	1:A:343:LYS:HZ2	1.71	0.56
2:B:535:GLY:O	2:B:536:GLU:HG3	2.05	0.56
2:B:287:VAL:HG13	2:B:290:SER:HB3	1.88	0.56
2:B:446:ALA:HB3	2:B:447:PRO:HD3	1.88	0.56
1:A:434:ALA:C	1:A:436:HIS:H	2.14	0.55
2:B:446:ALA:HB3	2:B:447:PRO:CD	2.35	0.55
3:A:4:HOH:O	2:B:460:CYS:CB	2.46	0.55
2:B:329:LYS:HB2	2:B:329:LYS:NZ	2.22	0.55
2:B:357:LYS:O	2:B:358:ALA:CB	2.54	0.55
2:B:408:ALA:O	2:B:412:LEU:HG	2.07	0.55
1:A:539:GLN:HE22	2:B:556:GLN:HE22	1.54	0.55
2:B:446:ALA:N	2:B:447:PRO:HD2	2.22	0.54
2:B:324:MET:HG3	2:B:343:LEU:C	2.32	0.54
1:A:373:VAL:O	1:A:376:GLN:HB3	2.07	0.54
2:B:482:TRP:CD1	2:B:501:VAL:HG22	2.43	0.54
1:A:433:ALA:O	1:A:437:LEU:HB2	2.08	0.54
2:B:359:LEU:HD21	2:B:361:LEU:HD11	1.90	0.54
1:A:370:VAL:CG2	1:A:380:PRO:HB2	2.38	0.53
1:A:389:TYR:OH	1:A:509:ASN:HB2	2.07	0.53
2:B:547:PRO:HD2	3:B:46:HOH:O	2.07	0.53
1:A:362:PHE:HB2	1:A:391:ILE:HB	1.91	0.53
1:A:479:LEU:O	1:A:483:TYR:HD1	1.91	0.53
1:A:396:MET:HG2	1:A:431:GLY:CA	2.34	0.53
1:A:339:GLN:HG3	1:A:343:LYS:NZ	2.24	0.52
2:B:365:ASP:O	2:B:366:GLN:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:VAL:HG22	2:B:549:LEU:HD11	1.91	0.52
2:B:325:ILE:HG13	2:B:326:ASP:H	1.72	0.52
2:B:543:ARG:HA	3:B:38:HOH:O	2.09	0.52
1:A:319:TYR:CD1	1:A:319:TYR:C	2.88	0.52
2:B:312:VAL:HG23	2:B:357:LYS:HB3	1.92	0.51
2:B:315:LEU:HD13	2:B:316:LEU:N	2.24	0.51
2:B:322:VAL:HA	2:B:325:ILE:CD1	2.40	0.51
1:A:484:GLN:HE21	1:A:484:GLN:CA	2.13	0.51
2:B:276:MET:HE2	2:B:437:CYS:SG	2.51	0.51
2:B:347:VAL:O	2:B:350:ILE:HB	2.11	0.51
1:A:370:VAL:HG21	1:A:380:PRO:HB2	1.93	0.51
1:A:599:ARG:HG3	1:A:599:ARG:HH11	1.76	0.51
2:B:310:PRO:O	2:B:311:THR:O	2.29	0.51
1:A:344:GLU:HA	1:A:347:ARG:HD3	1.92	0.51
1:A:514:LEU:N	1:A:514:LEU:HD23	2.26	0.51
1:A:568:TYR:HD1	1:A:577:LYS:HB3	1.75	0.51
2:B:346:PHE:HB3	3:B:23:HOH:O	2.10	0.51
2:B:409:GLU:HG2	3:B:8:HOH:O	2.11	0.51
2:B:495:GLU:HG3	3:B:2:HOH:O	2.10	0.51
1:A:432:SER:H	1:A:435:ALA:CB	2.24	0.50
2:B:324:MET:O	2:B:343:LEU:HD23	2.10	0.50
2:B:247:GLU:HA	2:B:250:LYS:CD	2.41	0.50
2:B:414:ASP:OD1	2:B:418:HIS:HD2	1.94	0.50
1:A:363:LEU:C	1:A:363:LEU:HD12	2.36	0.50
1:A:572:SER:OG	1:A:573:SER:N	2.44	0.50
1:A:612:SER:CA	3:A:17:HOH:O	2.59	0.50
2:B:315:LEU:HD13	2:B:316:LEU:H	1.76	0.50
2:B:326:ASP:O	2:B:327:ASN:C	2.55	0.50
2:B:406:VAL:HG23	2:B:407:ASP:N	2.26	0.50
1:A:428:GLU:CG	1:A:429:GLU:N	2.75	0.50
1:A:568:TYR:CD1	1:A:577:LYS:HB3	2.47	0.50
2:B:409:GLU:O	2:B:413:VAL:HG23	2.12	0.50
1:A:568:TYR:O	1:A:577:LYS:HE2	2.11	0.49
1:A:458:PHE:HA	2:B:422:GLN:OE1	2.13	0.49
2:B:349:ASP:O	2:B:353:LYS:HG3	2.12	0.49
2:B:446:ALA:H	2:B:447:PRO:HD2	1.77	0.49
1:A:344:GLU:OE2	1:A:466:LYS:HE3	2.12	0.49
2:B:535:GLY:O	2:B:536:GLU:CB	2.61	0.49
1:A:325:VAL:HG22	1:A:362:PHE:HE1	1.77	0.49
2:B:257:ASP:O	2:B:260:LEU:HB3	2.12	0.49
2:B:424:GLN:CG	2:B:425:ILE:N	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:LYS:HE3	2:B:430:LYS:CA	2.31	0.49
2:B:256:LEU:HD12	2:B:256:LEU:N	2.28	0.49
2:B:295:ARG:NH2	2:B:444:ALA:O	2.45	0.49
2:B:520:ASP:OD2	2:B:523:ARG:NH1	2.46	0.49
1:A:584:VAL:HB	1:A:593:LEU:HD12	1.95	0.49
1:A:463:GLN:O	1:A:464:ASP:HB3	2.11	0.49
1:A:540:LEU:HD13	1:A:554:VAL:HG11	1.94	0.49
2:B:510:LEU:HD22	2:B:514:TYR:CE2	2.48	0.48
1:A:339:GLN:O	1:A:340:GLU:C	2.57	0.48
1:A:376:GLN:O	1:A:376:GLN:HG3	2.13	0.48
2:B:318:ALA:O	2:B:322:VAL:HG23	2.12	0.48
2:B:295:ARG:NH1	2:B:309:GLU:OE1	2.47	0.48
1:A:542:GLN:NE2	2:B:484:ARG:HH21	2.12	0.48
1:A:319:TYR:CE2	1:A:488:LEU:HD13	2.48	0.48
1:A:462:VAL:CG1	1:A:463:GLN:N	2.77	0.48
2:B:313:LEU:HD11	2:B:362:VAL:HG21	1.95	0.48
1:A:532:VAL:HG21	2:B:559:THR:HG21	1.95	0.48
2:B:285:GLN:O	2:B:286:ALA:C	2.57	0.48
2:B:542:SER:O	2:B:543:ARG:CB	2.60	0.48
2:B:263:MET:HE1	2:B:315:LEU:HG	1.94	0.48
1:A:411:GLN:NE2	3:A:29:HOH:O	2.46	0.47
1:A:462:VAL:HG12	1:A:464:ASP:H	1.79	0.47
2:B:322:VAL:HA	2:B:325:ILE:HG12	1.97	0.47
2:B:365:ASP:O	2:B:366:GLN:CB	2.62	0.47
2:B:270:LEU:HD11	2:B:274:GLN:NE2	2.29	0.47
2:B:287:VAL:HG13	2:B:290:SER:CB	2.44	0.47
1:A:600:THR:HA	1:A:603:GLN:HE21	1.78	0.47
2:B:350:ILE:O	2:B:354:THR:N	2.48	0.47
1:A:410:GLU:O	1:A:413:PHE:HB3	2.15	0.47
2:B:311:THR:N	2:B:357:LYS:O	2.47	0.47
2:B:253:ILE:N	2:B:253:ILE:HD12	2.30	0.46
1:A:559:SER:HB2	2:B:562:PRO:CB	2.44	0.46
1:A:521:ASN:HD22	1:A:521:ASN:HA	1.54	0.46
1:A:323:LEU:HA	1:A:364:TRP:CD1	2.51	0.46
1:A:585:LYS:HA	1:A:591:ARG:O	2.15	0.46
2:B:523:ARG:HH11	2:B:523:ARG:HG3	1.79	0.46
1:A:388:ASP:CG	1:A:421:ARG:HH21	2.24	0.46
2:B:322:VAL:C	2:B:325:ILE:HG12	2.40	0.46
1:A:535:VAL:HG11	2:B:489:LEU:HD13	1.97	0.46
2:B:521:LYS:HB3	2:B:521:LYS:HZ2	1.81	0.46
2:B:324:MET:HA	2:B:342:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ARG:HG3	1:A:599:ARG:NH1	2.31	0.46
1:A:449:VAL:HG11	2:B:439:PHE:HA	1.98	0.46
2:B:312:VAL:CG2	2:B:357:LYS:CD	2.94	0.46
1:A:538:ARG:HD3	2:B:460:CYS:HB2	1.97	0.45
1:A:312:TRP:CD2	1:A:383:LYS:HD3	2.51	0.45
1:A:396:MET:HE3	1:A:430:CYS:CA	2.45	0.45
1:A:319:TYR:C	1:A:319:TYR:HD1	2.24	0.45
1:A:404:ILE:HD11	1:A:438:SER:HB3	1.97	0.45
1:A:346:GLN:HG3	1:A:352:PHE:HE1	1.82	0.45
2:B:289:CYS:HB3	2:B:315:LEU:HB3	1.98	0.45
1:A:391:ILE:HG12	1:A:424:ILE:HB	1.98	0.45
1:A:325:VAL:HG22	1:A:362:PHE:CE1	2.51	0.45
1:A:434:ALA:C	1:A:436:HIS:N	2.74	0.45
2:B:279:ARG:NH1	2:B:279:ARG:CB	2.76	0.45
2:B:312:VAL:HG23	2:B:357:LYS:CB	2.46	0.45
1:A:319:TYR:HE2	1:A:488:LEU:HD13	1.81	0.45
1:A:539:GLN:NE2	2:B:556:GLN:HE22	2.14	0.45
2:B:316:LEU:HD23	2:B:363:ILE:HG12	1.99	0.45
2:B:405:ARG:O	2:B:408:ALA:HB3	2.17	0.45
1:A:385:LEU:CD2	1:A:490:CYS:HB2	2.44	0.45
1:A:538:ARG:CD	2:B:460:CYS:HB2	2.47	0.45
2:B:366:GLN:CD	2:B:427:GLN:O	2.60	0.45
1:A:378:ARG:HH11	1:A:378:ARG:HG2	1.81	0.44
2:B:253:ILE:HD11	2:B:306:TRP:CZ2	2.51	0.44
2:B:521:LYS:HB3	2:B:521:LYS:HZ3	1.77	0.44
1:A:473:THR:OG1	1:A:474:ILE:N	2.51	0.44
1:A:461:ARG:HD3	3:A:37:HOH:O	2.18	0.44
2:B:441:LYS:O	2:B:444:ALA:HB3	2.18	0.44
1:A:373:VAL:HA	1:A:374:PRO:HD2	1.87	0.44
2:B:288:PRO:O	2:B:289:CYS:HB2	2.17	0.44
1:A:604:LEU:HD23	1:A:605:TYR:CE1	2.53	0.44
2:B:365:ASP:O	2:B:366:GLN:CG	2.65	0.44
1:A:550:LYS:HG2	1:A:586:TYR:CD2	2.52	0.44
1:A:559:SER:CB	2:B:562:PRO:HB3	2.45	0.44
1:A:341:LEU:HD23	1:A:341:LEU:C	2.43	0.44
1:A:481:LYS:HA	1:A:484:GLN:HG2	2.00	0.43
2:B:348:THR:O	2:B:351:THR:N	2.51	0.43
2:B:349:ASP:O	2:B:353:LYS:N	2.51	0.43
2:B:523:ARG:CZ	3:B:16:HOH:O	2.66	0.43
2:B:316:LEU:O	2:B:363:ILE:HA	2.19	0.43
2:B:535:GLY:O	2:B:536:GLU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ILE:CG2	2:B:413:VAL:HG21	2.48	0.43
1:A:544:SER:HB2	2:B:469:VAL:C	2.44	0.43
1:A:358:ASN:HB2	1:A:521:ASN:ND2	2.33	0.43
1:A:589:LEU:N	1:A:589:LEU:HD12	2.33	0.43
2:B:317:ARG:O	2:B:318:ALA:C	2.61	0.43
1:A:577:LYS:C	1:A:579:LYS:N	2.76	0.43
1:A:483:TYR:O	1:A:484:GLN:C	2.60	0.43
2:B:295:ARG:HG3	2:B:307:VAL:CG1	2.48	0.43
2:B:452:ARG:HG3	2:B:452:ARG:HH11	1.84	0.43
1:A:610:PRO:CB	2:B:505:PRO:HB2	2.49	0.43
2:B:311:THR:HG21	2:B:439:PHE:CE2	2.54	0.43
1:A:312:TRP:CD1	1:A:312:TRP:C	2.96	0.43
1:A:341:LEU:O	1:A:345:LEU:HB2	2.19	0.42
1:A:473:THR:O	1:A:476:THR:N	2.52	0.42
1:A:589:LEU:N	1:A:589:LEU:CD1	2.82	0.42
2:B:523:ARG:NH1	2:B:523:ARG:HG3	2.34	0.42
1:A:476:THR:O	1:A:480:GLN:HG3	2.19	0.42
1:A:610:PRO:HB3	2:B:505:PRO:CG	2.48	0.42
2:B:249:LEU:HD13	2:B:276:MET:HB3	2.01	0.42
2:B:273:LEU:HA	2:B:276:MET:HE3	2.01	0.42
2:B:310:PRO:O	2:B:357:LYS:HB3	2.18	0.42
1:A:488:LEU:N	1:A:488:LEU:CD1	2.83	0.42
2:B:260:LEU:HD12	2:B:263:MET:CE	2.49	0.42
2:B:321:PHE:C	2:B:323:SER:N	2.77	0.42
2:B:251:HIS:O	2:B:295:ARG:HA	2.19	0.42
1:A:353:ASP:OD2	1:A:355:ARG:NE	2.45	0.42
1:A:404:ILE:HG13	1:A:439:ILE:CD1	2.33	0.42
2:B:519:SER:C	2:B:523:ARG:NH1	2.78	0.42
1:A:531:THR:HG1	1:A:534:GLU:HG3	1.81	0.42
2:B:314:VAL:CG2	2:B:359:LEU:HD11	2.50	0.42
2:B:530:ILE:CA	2:B:534:ARG:HH12	2.18	0.42
2:B:549:LEU:HD22	2:B:553:ILE:HG13	2.01	0.42
1:A:439:ILE:HD12	1:A:439:ILE:H	1.84	0.42
1:A:509:ASN:ND2	2:B:417:LEU:O	2.52	0.42
1:A:530:GLN:HG3	2:B:490:ASN:ND2	2.35	0.42
1:A:595:PRO:HA	3:A:13:HOH:O	2.19	0.42
1:A:575:THR:O	1:A:579:LYS:HG3	2.19	0.41
2:B:287:VAL:HA	2:B:288:PRO:HD3	1.92	0.41
2:B:481:VAL:O	2:B:485:GLN:HG3	2.19	0.41
1:A:390:ILE:HB	1:A:420:LEU:HD23	2.01	0.41
1:A:487:THR:O	1:A:487:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:O	1:A:491:ARG:CD	2.67	0.41
1:A:400:CYS:SG	1:A:434:ALA:HB1	2.60	0.41
1:A:412:LYS:O	1:A:416:LYS:HG3	2.20	0.41
2:B:446:ALA:N	2:B:447:PRO:CD	2.84	0.41
1:A:474:ILE:HG22	2:B:413:VAL:HG21	2.03	0.41
1:A:517:PHE:O	1:A:520:PHE:HB3	2.20	0.41
2:B:524:GLN:C	2:B:525:ASN:HD22	2.29	0.41
2:B:548:GLU:HB2	3:B:46:HOH:O	2.21	0.41
1:A:343:LYS:HG3	1:A:344:GLU:N	2.34	0.41
2:B:321:PHE:C	2:B:323:SER:H	2.29	0.41
1:A:601:ILE:O	1:A:605:TYR:HD1	2.04	0.41
2:B:473:LEU:HD12	2:B:473:LEU:HA	1.95	0.41
1:A:542:GLN:HE22	2:B:484:ARG:HH21	1.68	0.40
2:B:309:GLU:HG3	2:B:310:PRO:CD	2.50	0.40
2:B:348:THR:O	2:B:349:ASP:C	2.64	0.40
1:A:359:VAL:O	1:A:359:VAL:HG13	2.20	0.40
2:B:451:LEU:HD12	2:B:454:GLU:OE2	2.20	0.40
1:A:428:GLU:C	1:A:430:CYS:N	2.70	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	275/311 (88%)	240 (87%)	26 (10%)	9 (3%)	3	7
2	B	246/341 (72%)	213 (87%)	24 (10%)	9 (4%)	2	6
All	All	521/652 (80%)	453 (87%)	50 (10%)	18 (4%)	3	6

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	GLU
1	A	430	CYS
1	A	432	SER
2	B	310	PRO
2	B	311	THR
2	B	358	ALA
1	A	380	PRO
1	A	484	GLN
1	A	580	LEU
2	B	286	ALA
2	B	327	ASN
2	B	366	GLN
2	B	543	ARG
1	A	436	HIS
1	A	435	ALA
2	B	318	ALA
2	B	505	PRO
1	A	381	VAL

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	247/271 (91%)	236 (96%)	11 (4%)	24	52
2	B	220/290 (76%)	197 (90%)	23 (10%)	6	17
All	All	467/561 (83%)	433 (93%)	34 (7%)	13	32

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	TRP
1	A	319	TYR
1	A	415	LEU
1	A	420	LEU
1	A	428	GLU
1	A	436	HIS

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Mol	Chain	Res	Type
1	A	484	GLN
1	A	514	LEU
1	A	521	ASN
1	A	526	LYS
1	A	554	VAL
2	B	269	LEU
2	B	274	GLN
2	B	279	ARG
2	B	287	VAL
2	B	291	VAL
2	B	306	TRP
2	B	311	THR
2	B	315	LEU
2	B	329	LYS
2	B	351	THR
2	B	364	VAL
2	B	422	GLN
2	B	424	GLN
2	B	430	LYS
2	B	432	LEU
2	B	452	ARG
2	B	473	LEU
2	B	489	LEU
2	B	501	VAL
2	B	509	LEU
2	B	510	LEU
2	B	521	LYS
2	B	549	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	GLN
1	A	358	ASN
1	A	376	GLN
1	A	411	GLN
1	A	445	GLN
1	A	446	GLN
1	A	450	ASN
1	A	463	GLN
1	A	484	GLN
1	A	521	ASN

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Mol	Chain	Res	Type
1	A	539	GLN
1	A	542	GLN
1	A	557	HIS
1	A	603	GLN
2	B	268	GLN
2	B	274	GLN
2	B	285	GLN
2	B	327	ASN
2	B	416	GLN
2	B	418	HIS
2	B	424	GLN
2	B	508	GLN
2	B	512	GLN
2	B	524	GLN
2	B	525	ASN
2	B	531	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 [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	281/311 (90%)	-0.02	8 (2%) 55 51	23, 48, 77, 95	0
2	B	258/341 (75%)	0.14	10 (3%) 43 39	19, 52, 91, 103	0
All	All	539/652 (82%)	0.06	18 (3%) 49 45	19, 50, 87, 103	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	ALA	3.8
2	B	532	VAL	3.3
2	B	446	ALA	3.0
2	B	320	ALA	2.8
2	B	541	THR	2.8
1	A	508	ALA	2.7
2	B	451	LEU	2.6
2	B	447	PRO	2.6
1	A	377	LEU	2.5
1	A	331	THR	2.5
2	B	278	CYS	2.3
1	A	430	CYS	2.3
2	B	306	TRP	2.3
1	A	332	GLY	2.3
1	A	436	HIS	2.2
1	A	434	ALA	2.1
2	B	318	ALA	2.1
2	B	367	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.