Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 12:57 PM EST

PDB ID	:	2ZIV
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	:	2.70 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 (i) 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 (1)) were used in the production of this report:

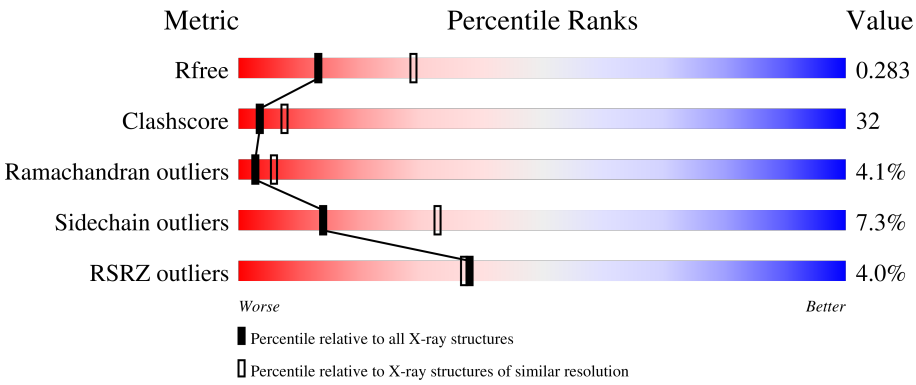
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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%; 47%; 39%; 5%; 10%
2	B	351	2%; 38%; 31%; 7%; •; 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4425 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
			Total	C	N	O	S			
1	A	281	2227	1409	392	411	15	0	0	0

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
			Total	C	N	O	S			
2	B	269	2108	1328	369	399	12	0	0	0

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.

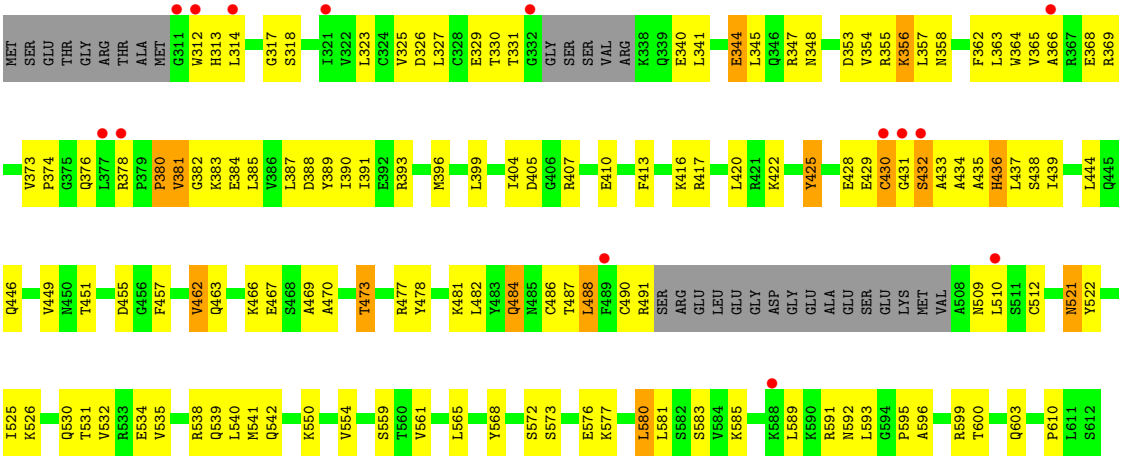
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	49	49	49	0	0
			Total	O		
3	B	41	41	41	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

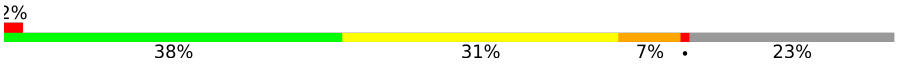
• Molecule 1: Mus81 protein

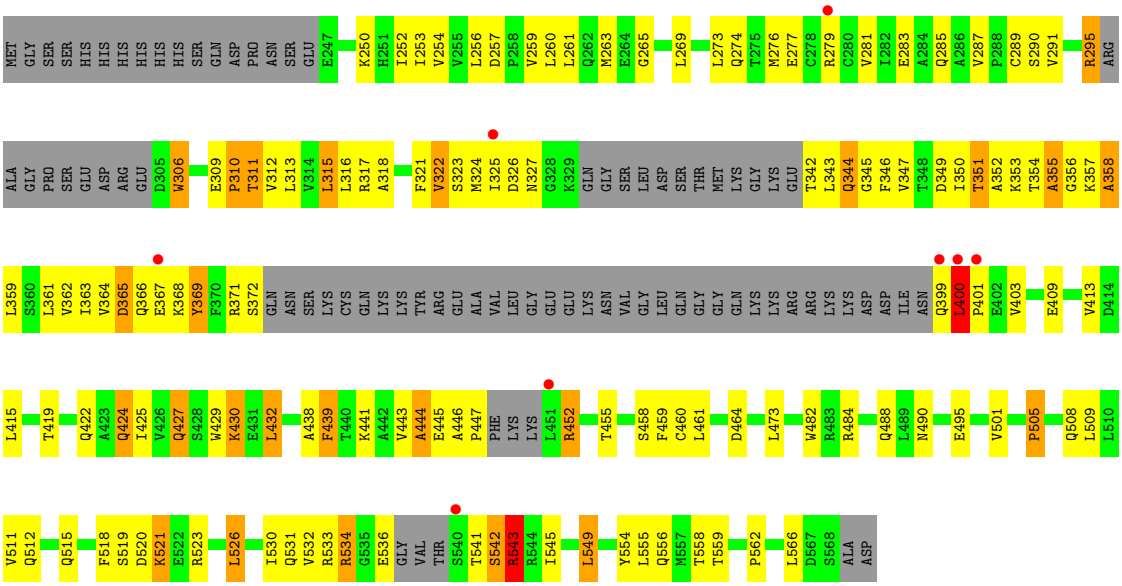
Chain A:



• Molecule 2: Crossover junction endonuclease EME1

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.44Å 88.44Å 169.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.50 – 2.70 45.50 – 2.52	Depositor EDS
% Data completeness (in resolution range)	96.2 (45.50-2.70) 98.8 (45.50-2.52)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.278 0.234 , 0.283	Depositor DCC
R_{free} test set	1043 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4425	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.39	0/2262	0.60	0/3045
2	B	0.39	0/2136	0.63	0/2890
All	All	0.39	0/4398	0.62	0/5935

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	2227	0	2276	136	0
2	B	2108	0	2126	159	0
3	A	49	0	0	6	0
3	B	41	0	0	10	0
All	All	4425	0	4402	280	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 32.

All (280) 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)
2:B:351:THR:HA	2:B:354:THR:HG22	1.32	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:LYS:HA	2:B:430:LYS:HE3	1.44	0.95
2:B:531:GLN:H	2:B:534:ARG:HE	1.02	0.93
2:B:455:THR:HG23	2:B:458:SER:H	1.35	0.89
2:B:531:GLN:N	2:B:534:ARG:HE	1.73	0.86
2:B:531:GLN:H	2:B:534:ARG:NE	1.75	0.83
1:A:559:SER:HB2	2:B:562:PRO:HB3	1.60	0.83
1:A:484:GLN:HE21	1:A:484:GLN:HA	1.47	0.79
2:B:250:LYS:HE2	2:B:277:GLU:OE1	1.83	0.79
1:A:358:ASN:H	1:A:521:ASN:HD21	1.29	0.78
2:B:543:ARG:HA	2:B:543:ARG:NE	1.99	0.78
2:B:326:ASP:OD2	2:B:401:PRO:HG2	1.84	0.78
1:A:434:ALA:HA	1:A:437:LEU:HB3	1.64	0.77
1:A:462:VAL:HG13	1:A:467:GLU:HB3	1.67	0.76
1:A:482:LEU:HD13	1:A:510:LEU:HD11	1.66	0.76
1:A:522:TYR:O	1:A:525:ILE:HG22	1.86	0.75
2:B:533:ARG:HD2	3:B:16:HOH:O	1.87	0.74
1:A:568:TYR:O	1:A:577:LYS:HE2	1.87	0.74
1:A:542:GLN:HE21	2:B:484:ARG:HE	1.36	0.73
2:B:351:THR:HA	2:B:354:THR:CG2	2.15	0.72
1:A:362:PHE:HB2	1:A:391:ILE:HB	1.72	0.72
1:A:600:THR:HA	1:A:603:GLN:HE21	1.55	0.71
1:A:385:LEU:HD21	1:A:490:CYS:HB2	1.71	0.71
1:A:326:ASP:HB2	1:A:357:LEU:HD12	1.72	0.70
1:A:422:LYS:HE3	1:A:509:ASN:HB3	1.74	0.69
2:B:555:LEU:O	2:B:559:THR:HG22	1.93	0.69
1:A:599:ARG:HG3	1:A:599:ARG:HH11	1.57	0.69
2:B:351:THR:CA	2:B:354:THR:HG22	2.16	0.69
1:A:428:GLU:C	1:A:430:CYS:H	1.96	0.68
1:A:385:LEU:HD12	1:A:488:LEU:HD23	1.75	0.68
2:B:252:ILE:HD13	2:B:295:ARG:HB3	1.75	0.68
1:A:404:ILE:HD11	1:A:438:SER:HB2	1.76	0.68
1:A:390:ILE:HB	1:A:420:LEU:HD23	1.77	0.67
1:A:365:VAL:CG2	1:A:384:GLU:HB3	2.25	0.67
1:A:488:LEU:H	1:A:488:LEU:HD22	1.60	0.66
1:A:522:TYR:CZ	1:A:526:LYS:HD2	2.31	0.66
1:A:341:LEU:O	1:A:345:LEU:HB2	1.95	0.66
2:B:260:LEU:HD12	2:B:263:MET:CE	2.26	0.66
1:A:344:GLU:HG3	1:A:466:LYS:HG3	1.77	0.65
1:A:531:THR:OG1	1:A:534:GLU:HG3	1.95	0.65
1:A:599:ARG:O	1:A:603:GLN:HG3	1.96	0.65
1:A:404:ILE:HG13	1:A:439:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:LEU:HA	2:B:263:MET:HE2	1.78	0.65
1:A:542:GLN:NE2	2:B:484:ARG:HE	1.95	0.64
2:B:363:ILE:HB	2:B:425:ILE:HG12	1.80	0.64
1:A:364:TRP:HB2	1:A:387:LEU:HD22	1.79	0.63
1:A:354:VAL:O	1:A:354:VAL:HG12	1.99	0.63
2:B:366:GLN:HA	2:B:427:GLN:O	1.99	0.63
1:A:365:VAL:HG21	1:A:384:GLU:HB3	1.80	0.63
2:B:446:ALA:N	2:B:447:PRO:HD2	2.12	0.63
2:B:253:ILE:HG13	2:B:279:ARG:NH1	2.14	0.63
2:B:279:ARG:HH11	2:B:279:ARG:HB3	1.62	0.63
2:B:346:PHE:O	2:B:350:ILE:HG13	1.99	0.63
1:A:430:CYS:SG	1:A:463:GLN:HG3	2.40	0.62
2:B:263:MET:HG2	2:B:317:ARG:HH12	1.64	0.62
2:B:313:LEU:HD11	2:B:362:VAL:HG23	1.81	0.61
2:B:357:LYS:O	2:B:358:ALA:HB3	2.00	0.61
1:A:484:GLN:HE21	1:A:484:GLN:CA	2.13	0.61
1:A:491:ARG:HD3	1:A:491:ARG:C	2.21	0.61
1:A:329:GLU:HG2	1:A:362:PHE:CZ	2.36	0.60
2:B:312:VAL:HG23	2:B:357:LYS:HB3	1.83	0.60
1:A:589:LEU:HB2	1:A:591:ARG:NE	2.17	0.60
2:B:357:LYS:O	2:B:358:ALA:CB	2.50	0.60
2:B:554:TYR:O	2:B:558:THR:HB	2.02	0.60
2:B:521:LYS:NZ	2:B:521:LYS:HB3	2.17	0.60
2:B:315:LEU:HD11	2:B:364:VAL:CG2	2.32	0.60
2:B:534:ARG:HH11	2:B:534:ARG:HG2	1.67	0.60
2:B:536:GLU:OE1	2:B:536:GLU:HA	2.01	0.60
2:B:343:LEU:C	2:B:345:GLY:H	2.05	0.60
2:B:542:SER:O	2:B:543:ARG:HB2	2.02	0.59
1:A:434:ALA:C	1:A:436:HIS:H	2.06	0.59
2:B:257:ASP:OD2	2:B:259:VAL:HG22	2.02	0.59
2:B:318:ALA:HB2	2:B:365:ASP:HB3	1.84	0.59
2:B:365:ASP:CG	2:B:365:ASP:O	2.41	0.59
2:B:495:GLU:CD	3:B:16:HOH:O	2.42	0.58
1:A:396:MET:HG2	1:A:431:GLY:HA2	1.86	0.58
2:B:315:LEU:HD11	2:B:364:VAL:HG21	1.86	0.58
1:A:595:PRO:HG2	1:A:596:ALA:H	1.69	0.58
2:B:346:PHE:CZ	2:B:350:ILE:HD11	2.39	0.57
2:B:309:GLU:HG2	2:B:443:VAL:HG13	1.85	0.57
1:A:583:SER:HA	1:A:592:ASN:HD22	1.69	0.57
2:B:256:LEU:HD22	2:B:261:LEU:HD21	1.86	0.57
2:B:445:GLU:N	2:B:445:GLU:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:ILE:HD11	2:B:403:VAL:HG21	1.85	0.57
1:A:432:SER:H	1:A:435:ALA:HB2	1.69	0.57
1:A:491:ARG:HD3	1:A:491:ARG:O	2.05	0.57
2:B:495:GLU:HG2	3:B:16:HOH:O	2.05	0.56
1:A:432:SER:H	1:A:435:ALA:CB	2.19	0.56
1:A:599:ARG:HG3	1:A:599:ARG:NH1	2.17	0.56
2:B:310:PRO:O	2:B:311:THR:O	2.23	0.56
2:B:313:LEU:HD11	2:B:362:VAL:CG2	2.36	0.56
2:B:253:ILE:HG13	2:B:279:ARG:HH11	1.71	0.56
1:A:344:GLU:HG2	1:A:347:ARG:NH1	2.20	0.56
2:B:322:VAL:HG12	2:B:322:VAL:O	2.06	0.56
2:B:543:ARG:HG3	3:B:90:HOH:O	2.05	0.55
2:B:260:LEU:HD12	2:B:263:MET:HE1	1.87	0.55
2:B:530:ILE:HA	2:B:534:ARG:NH2	2.21	0.55
1:A:541:MET:HE1	2:B:460:CYS:O	2.07	0.55
1:A:344:GLU:HA	1:A:347:ARG:HD3	1.87	0.55
2:B:315:LEU:HD13	2:B:316:LEU:H	1.72	0.55
2:B:357:LYS:NZ	3:B:38:HOH:O	2.38	0.55
2:B:279:ARG:NH1	2:B:279:ARG:HB3	2.21	0.55
1:A:364:TRP:CB	1:A:387:LEU:HD22	2.35	0.55
1:A:478:TYR:O	1:A:482:LEU:HG	2.07	0.55
1:A:541:MET:HE1	2:B:461:LEU:HA	1.89	0.55
1:A:368:GLU:HB3	1:A:382:GLY:HA3	1.89	0.55
2:B:324:MET:SD	2:B:344:GLN:HA	2.47	0.55
2:B:349:ASP:HA	2:B:352:ALA:HB3	1.89	0.54
1:A:585:LYS:NZ	1:A:592:ASN:HD21	2.05	0.54
2:B:322:VAL:HG13	2:B:403:VAL:CG2	2.38	0.54
2:B:318:ALA:HB2	2:B:365:ASP:CB	2.38	0.54
2:B:366:GLN:CD	2:B:366:GLN:H	2.11	0.54
1:A:399:LEU:HD23	1:A:444:LEU:HD22	1.89	0.54
1:A:585:LYS:HA	1:A:591:ARG:O	2.08	0.54
2:B:315:LEU:HD21	2:B:432:LEU:HD11	1.90	0.53
1:A:365:VAL:HG23	1:A:385:LEU:O	2.07	0.53
2:B:325:ILE:HG13	2:B:326:ASP:N	2.24	0.53
1:A:484:GLN:HA	1:A:484:GLN:NE2	2.20	0.53
2:B:521:LYS:HB3	2:B:521:LYS:HZ2	1.74	0.53
2:B:543:ARG:HG3	2:B:543:ARG:HH11	1.74	0.53
2:B:354:THR:O	2:B:355:ALA:C	2.47	0.52
1:A:388:ASP:O	1:A:422:LYS:HB2	2.09	0.52
1:A:428:GLU:C	1:A:430:CYS:N	2.63	0.52
1:A:580:LEU:HG	1:A:581:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:THR:N	2:B:357:LYS:O	2.42	0.51
2:B:482:TRP:CD1	2:B:501:VAL:HG22	2.45	0.51
2:B:321:PHE:C	2:B:323:SER:H	2.12	0.51
1:A:383:LYS:HB2	1:A:383:LYS:NZ	2.26	0.51
1:A:405:ASP:OD1	1:A:407:ARG:NH1	2.44	0.51
1:A:451:THR:HA	1:A:455:ASP:OD2	2.10	0.51
1:A:535:VAL:O	1:A:539:GLN:HG3	2.11	0.51
1:A:374:PRO:HG2	3:A:27:HOH:O	2.11	0.50
2:B:281:VAL:HG12	2:B:283:GLU:HG3	1.94	0.50
2:B:368:LYS:O	2:B:371:ARG:HB2	2.10	0.50
1:A:530:GLN:HG3	2:B:490:ASN:ND2	2.27	0.50
1:A:373:VAL:O	1:A:376:GLN:HG2	2.12	0.50
1:A:573:SER:HB3	1:A:576:GLU:HB2	1.94	0.50
2:B:511:VAL:O	2:B:515:GLN:HG2	2.12	0.50
2:B:285:GLN:HG3	2:B:290:SER:O	2.11	0.50
1:A:348:ASN:OD1	1:A:473:THR:HG21	2.12	0.49
1:A:540:LEU:HD13	1:A:554:VAL:HG11	1.93	0.49
2:B:321:PHE:O	2:B:323:SER:N	2.38	0.49
1:A:327:LEU:HD23	1:A:354:VAL:HG12	1.93	0.49
2:B:399:GLN:O	2:B:400:LEU:O	2.30	0.49
2:B:430:LYS:HE3	2:B:430:LYS:CA	2.31	0.49
2:B:309:GLU:HG3	2:B:310:PRO:HD2	1.94	0.49
1:A:404:ILE:HD11	1:A:438:SER:CB	2.42	0.49
2:B:534:ARG:HG2	2:B:534:ARG:NH1	2.28	0.49
1:A:446:GLN:NE2	2:B:438:ALA:HA	2.28	0.49
2:B:455:THR:HG22	2:B:458:SER:HB2	1.94	0.49
2:B:531:GLN:CB	2:B:534:ARG:HE	2.25	0.49
2:B:359:LEU:HD21	2:B:361:LEU:HD11	1.93	0.49
1:A:466:LYS:O	1:A:469:ALA:HB3	2.13	0.48
2:B:306:TRP:HA	2:B:306:TRP:CE3	2.48	0.48
2:B:354:THR:O	2:B:354:THR:HG23	2.13	0.48
2:B:363:ILE:HD12	2:B:425:ILE:HG12	1.95	0.48
1:A:559:SER:HB2	2:B:562:PRO:CB	2.37	0.48
1:A:532:VAL:HG21	2:B:559:THR:HG21	1.96	0.48
1:A:369:ARG:HA	3:A:14:HOH:O	2.13	0.48
2:B:263:MET:HG2	2:B:317:ARG:NH1	2.28	0.47
2:B:508:GLN:O	2:B:512:GLN:HG2	2.14	0.47
2:B:520:ASP:OD2	2:B:523:ARG:NH1	2.47	0.47
1:A:434:ALA:C	1:A:436:HIS:N	2.67	0.47
2:B:343:LEU:C	2:B:345:GLY:N	2.68	0.47
2:B:409:GLU:O	2:B:413:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:GLN:HG2	3:B:29:HOH:O	2.14	0.47
2:B:445:GLU:O	2:B:445:GLU:HG2	2.14	0.47
1:A:353:ASP:OD2	1:A:355:ARG:NE	2.38	0.47
1:A:486:CYS:HB3	1:A:512:CYS:SG	2.54	0.47
2:B:536:GLU:HG2	3:B:55:HOH:O	2.14	0.47
2:B:518:PHE:O	2:B:519:SER:HB3	2.15	0.47
1:A:429:GLU:O	1:A:431:GLY:N	2.48	0.47
2:B:526:LEU:HG	2:B:526:LEU:O	2.15	0.47
1:A:344:GLU:CG	1:A:466:LYS:HG3	2.44	0.46
1:A:462:VAL:CG1	1:A:463:GLN:N	2.79	0.46
1:A:429:GLU:OE2	1:A:432:SER:HB2	2.15	0.46
2:B:265:GLY:HA3	2:B:429:TRP:CD2	2.50	0.46
2:B:543:ARG:HG3	2:B:543:ARG:NH1	2.31	0.46
1:A:572:SER:OG	1:A:573:SER:N	2.49	0.46
1:A:432:SER:N	1:A:435:ALA:HB2	2.31	0.46
2:B:542:SER:O	2:B:543:ARG:CB	2.64	0.46
1:A:387:LEU:HB2	3:A:39:HOH:O	2.14	0.45
2:B:343:LEU:O	2:B:345:GLY:N	2.49	0.45
2:B:347:VAL:HA	2:B:350:ILE:HD12	1.97	0.45
2:B:473:LEU:HD22	2:B:473:LEU:H	1.80	0.45
2:B:545:ILE:HG23	2:B:549:LEU:HD13	1.97	0.45
1:A:589:LEU:HB2	1:A:591:ARG:HE	1.81	0.45
2:B:257:ASP:O	2:B:260:LEU:HB3	2.16	0.45
1:A:481:LYS:HA	1:A:484:GLN:HG2	1.98	0.45
2:B:452:ARG:HG3	2:B:452:ARG:HH11	1.81	0.45
1:A:330:THR:OG1	1:A:331:THR:N	2.50	0.45
1:A:603:GLN:NE2	3:A:57:HOH:O	2.40	0.45
1:A:522:TYR:O	1:A:526:LYS:HG3	2.15	0.45
2:B:254:VAL:HG11	2:B:273:LEU:HD13	1.99	0.45
2:B:273:LEU:HA	2:B:276:MET:HE2	1.98	0.44
2:B:446:ALA:N	2:B:447:PRO:CD	2.75	0.44
2:B:484:ARG:O	2:B:488:GLN:HG2	2.17	0.44
1:A:313:HIS:ND1	1:A:313:HIS:C	2.71	0.44
1:A:532:VAL:HG22	2:B:566:LEU:HD21	1.99	0.44
2:B:324:MET:HA	2:B:342:THR:O	2.17	0.44
2:B:531:GLN:HB2	2:B:534:ARG:HE	1.81	0.44
2:B:295:ARG:HH11	2:B:295:ARG:HG2	1.82	0.44
2:B:324:MET:HA	2:B:327:ASN:ND2	2.33	0.44
1:A:378:ARG:HH11	1:A:378:ARG:HG2	1.83	0.44
1:A:389:TYR:OH	1:A:509:ASN:HB2	2.17	0.44
1:A:572:SER:HB3	3:A:46:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:THR:HA	2:B:358:ALA:HB3	2.00	0.44
1:A:317:GLY:O	1:A:369:ARG:NH1	2.46	0.44
1:A:365:VAL:HG22	1:A:366:ALA:N	2.32	0.44
1:A:363:LEU:C	1:A:363:LEU:HD12	2.37	0.44
2:B:253:ILE:N	2:B:253:ILE:HD12	2.32	0.44
2:B:415:LEU:HD23	2:B:419:THR:OG1	2.17	0.44
1:A:457:PHE:CD1	1:A:457:PHE:N	2.86	0.43
1:A:438:SER:OG	1:A:439:ILE:N	2.50	0.43
1:A:610:PRO:CB	2:B:505:PRO:HB2	2.48	0.43
1:A:449:VAL:HG11	2:B:439:PHE:HA	2.00	0.43
2:B:349:ASP:O	2:B:353:LYS:N	2.46	0.43
1:A:356:LYS:HE3	1:A:356:LYS:HA	2.00	0.43
2:B:531:GLN:CA	2:B:534:ARG:HE	2.30	0.43
1:A:329:GLU:OE2	1:A:393:ARG:HD3	2.19	0.43
1:A:488:LEU:HD22	1:A:488:LEU:N	2.31	0.43
2:B:369:TYR:CD1	2:B:369:TYR:C	2.91	0.43
1:A:425:TYR:HD2	1:A:457:PHE:HD2	1.66	0.43
1:A:538:ARG:NH2	2:B:464:ASP:OD1	2.51	0.43
2:B:322:VAL:HG13	2:B:403:VAL:HG21	2.00	0.43
1:A:429:GLU:HG2	1:A:431:GLY:O	2.19	0.42
2:B:363:ILE:HD12	2:B:425:ILE:CG1	2.49	0.42
1:A:410:GLU:HA	2:B:459:PHE:CZ	2.54	0.42
2:B:441:LYS:O	2:B:444:ALA:HB3	2.19	0.42
1:A:413:PHE:HA	1:A:416:LYS:HD2	2.00	0.42
1:A:429:GLU:O	1:A:429:GLU:HG2	2.19	0.42
2:B:252:ILE:HG13	2:B:444:ALA:HA	2.01	0.42
2:B:347:VAL:O	2:B:351:THR:OG1	2.37	0.42
1:A:477:ARG:O	1:A:481:LYS:HD3	2.19	0.42
2:B:324:MET:HG3	2:B:343:LEU:C	2.39	0.42
2:B:495:GLU:CG	3:B:16:HOH:O	2.63	0.42
2:B:556:GLN:NE2	3:B:30:HOH:O	2.52	0.42
2:B:399:GLN:C	2:B:400:LEU:HG	2.39	0.42
2:B:430:LYS:HA	2:B:430:LYS:CE	2.29	0.42
2:B:306:TRP:HA	2:B:306:TRP:HE3	1.84	0.42
2:B:318:ALA:O	2:B:322:VAL:HG23	2.20	0.42
2:B:367:GLU:H	2:B:367:GLU:HG2	1.62	0.42
1:A:470:ALA:O	1:A:473:THR:HG23	2.19	0.42
2:B:279:ARG:NH1	2:B:279:ARG:CB	2.82	0.42
2:B:315:LEU:HD13	2:B:316:LEU:N	2.33	0.42
2:B:321:PHE:C	2:B:323:SER:N	2.73	0.42
2:B:531:GLN:O	2:B:534:ARG:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:VAL:O	1:A:354:VAL:HA	2.20	0.42
1:A:380:PRO:O	1:A:381:VAL:HB	2.20	0.42
1:A:457:PHE:N	1:A:457:PHE:HD1	2.18	0.42
1:A:481:LYS:O	1:A:484:GLN:HG2	2.20	0.42
2:B:315:LEU:HD11	2:B:364:VAL:HG23	2.01	0.42
1:A:314:LEU:HB2	1:A:488:LEU:CD2	2.49	0.41
1:A:389:TYR:CE1	1:A:422:LYS:HG3	2.55	0.41
1:A:550:LYS:HB3	1:A:593:LEU:HD21	2.01	0.41
1:A:585:LYS:HZ1	1:A:592:ASN:HD21	1.68	0.41
2:B:325:ILE:CG1	2:B:326:ASP:N	2.82	0.41
1:A:318:SER:O	1:A:369:ARG:HG3	2.20	0.41
2:B:530:ILE:O	2:B:545:ILE:HG12	2.21	0.41
1:A:330:THR:HG21	1:A:354:VAL:HG11	2.03	0.41
1:A:561:VAL:O	1:A:565:LEU:HG	2.21	0.41
1:A:323:LEU:HD21	1:A:345:LEU:HD21	2.03	0.41
1:A:462:VAL:HG13	1:A:463:GLN:N	2.36	0.41
1:A:610:PRO:HB3	2:B:505:PRO:HB2	2.02	0.41
2:B:371:ARG:O	2:B:372:SER:HB2	2.21	0.41
1:A:358:ASN:H	1:A:521:ASN:ND2	2.07	0.41
1:A:568:TYR:CD1	1:A:577:LYS:HB3	2.56	0.41
1:A:585:LYS:HE3	1:A:592:ASN:OD1	2.21	0.41
2:B:312:VAL:HG21	2:B:354:THR:OG1	2.19	0.41
1:A:387:LEU:HD12	1:A:387:LEU:N	2.36	0.41
1:A:595:PRO:HD2	3:A:21:HOH:O	2.21	0.41
2:B:519:SER:O	2:B:523:ARG:HG3	2.21	0.41
2:B:515:GLN:HA	2:B:515:GLN:OE1	2.22	0.40
1:A:488:LEU:N	1:A:488:LEU:HD13	2.36	0.40
2:B:532:VAL:HG11	3:B:51:HOH:O	2.21	0.40
2:B:536:GLU:OE1	2:B:536:GLU:CA	2.68	0.40
1:A:431:GLY:HA2	1:A:435:ALA:HB2	2.04	0.40
1:A:327:LEU:HG	1:A:355:ARG:O	2.20	0.40
2:B:346:PHE:CE2	2:B:350:ILE:HD11	2.57	0.40
2:B:455:THR:CG2	2:B:458:SER:HB2	2.52	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	275/311 (88%)	245 (89%)	22 (8%)	8 (3%)	4 10
2	B	257/351 (73%)	225 (88%)	18 (7%)	14 (5%)	2 3
All	All	532/662 (80%)	470 (88%)	40 (8%)	22 (4%)	3 6

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	430	CYS
1	A	432	SER
2	B	310	PRO
2	B	311	THR
2	B	355	ALA
2	B	358	ALA
2	B	542	SER
1	A	340	GLU
1	A	436	HIS
2	B	322	VAL
2	B	344	GLN
2	B	526	LEU
1	A	433	ALA
1	A	580	LEU
2	B	400	LEU
2	B	444	ALA
2	B	543	ARG
1	A	381	VAL
2	B	505	PRO
2	B	541	THR
2	B	356	GLY
1	A	380	PRO

5.3.2 Protein sidechains (i)

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%)	27 55
2	B	231/301 (77%)	207 (90%)	24 (10%)	7 16
All	All	478/572 (84%)	443 (93%)	35 (7%)	14 33

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	TRP
1	A	344	GLU
1	A	356	LYS
1	A	417	ARG
1	A	425	TYR
1	A	462	VAL
1	A	473	THR
1	A	484	GLN
1	A	487	THR
1	A	488	LEU
1	A	521	ASN
2	B	269	LEU
2	B	274	GLN
2	B	287	VAL
2	B	289	CYS
2	B	291	VAL
2	B	295	ARG
2	B	306	TRP
2	B	315	LEU
2	B	351	THR
2	B	365	ASP
2	B	369	TYR
2	B	400	LEU
2	B	422	GLN
2	B	424	GLN
2	B	427	GLN
2	B	430	LYS

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Mol	Chain	Res	Type
2	B	432	LEU
2	B	439	PHE
2	B	452	ARG
2	B	509	LEU
2	B	521	LYS
2	B	534	ARG
2	B	543	ARG
2	B	549	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	GLN
1	A	411	GLN
1	A	446	GLN
1	A	450	ASN
1	A	452	GLN
1	A	463	GLN
1	A	480	GLN
1	A	484	GLN
1	A	521	ASN
1	A	539	GLN
1	A	542	GLN
1	A	592	ASN
1	A	603	GLN
2	B	251	HIS
2	B	274	GLN
2	B	327	ASN
2	B	366	GLN
2	B	416	GLN
2	B	418	HIS
2	B	422	GLN
2	B	424	GLN
2	B	485	GLN
2	B	524	GLN
2	B	525	ASN
2	B	531	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (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%)	0.09	14 (4%)	28	27	32, 56, 89, 108	0
2	B	269/351 (76%)	0.05	8 (2%)	50	51	28, 56, 95, 107	0
All	All	550/662 (83%)	0.07	22 (4%)	38	37	28, 56, 92, 108	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	451	LEU	6.3
2	B	400	LEU	5.6
2	B	540	SER	4.9
1	A	489	PHE	4.4
1	A	377	LEU	3.8
1	A	312	TRP	3.8
1	A	311	GLY	3.6
1	A	366	ALA	3.1
1	A	321	ILE	3.0
2	B	401	PRO	2.9
1	A	431	GLY	2.7
1	A	332	GLY	2.5
2	B	399	GLN	2.5
2	B	367	GLU	2.4
2	B	279	ARG	2.3
1	A	314	LEU	2.3
1	A	432	SER	2.2
1	A	430	CYS	2.2
1	A	378	ARG	2.1
1	A	588	LYS	2.1
2	B	325	ILE	2.1
1	A	510	LEU	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 monosaccharides 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.