Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:05 AM GMT

PDB ID	:	2ZIW
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

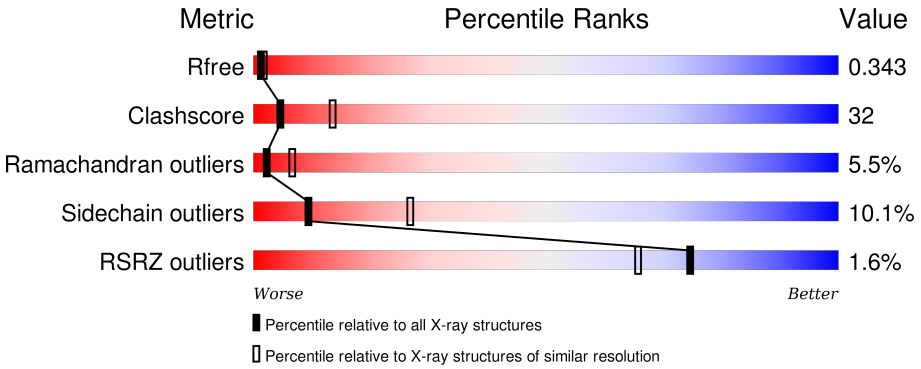
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	2% 45% 34% 7% • 13%
2	B	341	% 33% 27% 6% 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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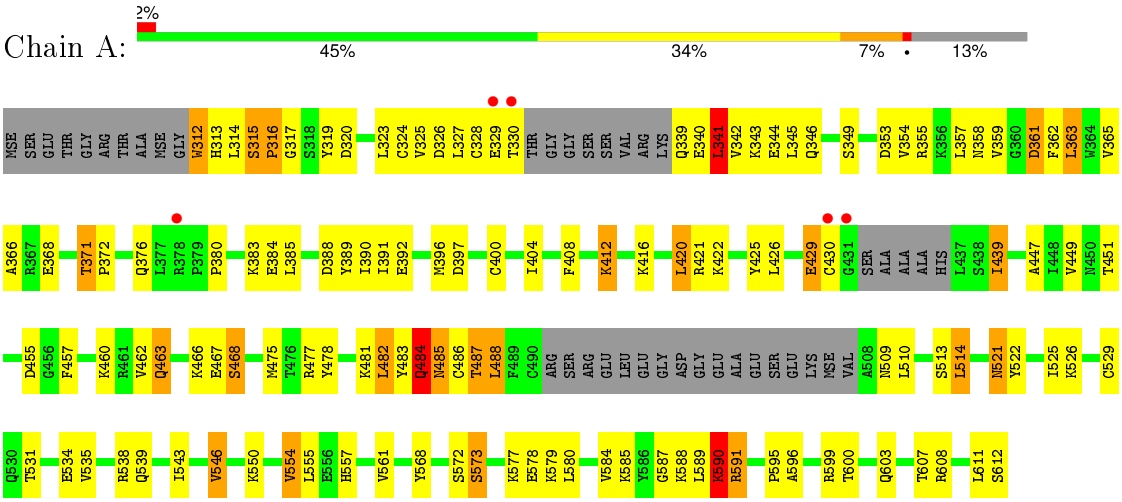
Chain	Residue	Modelled	Actual	Comment	Reference
B	245	SER	-	EXPRESSION TAG	UNP Q96AY2

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

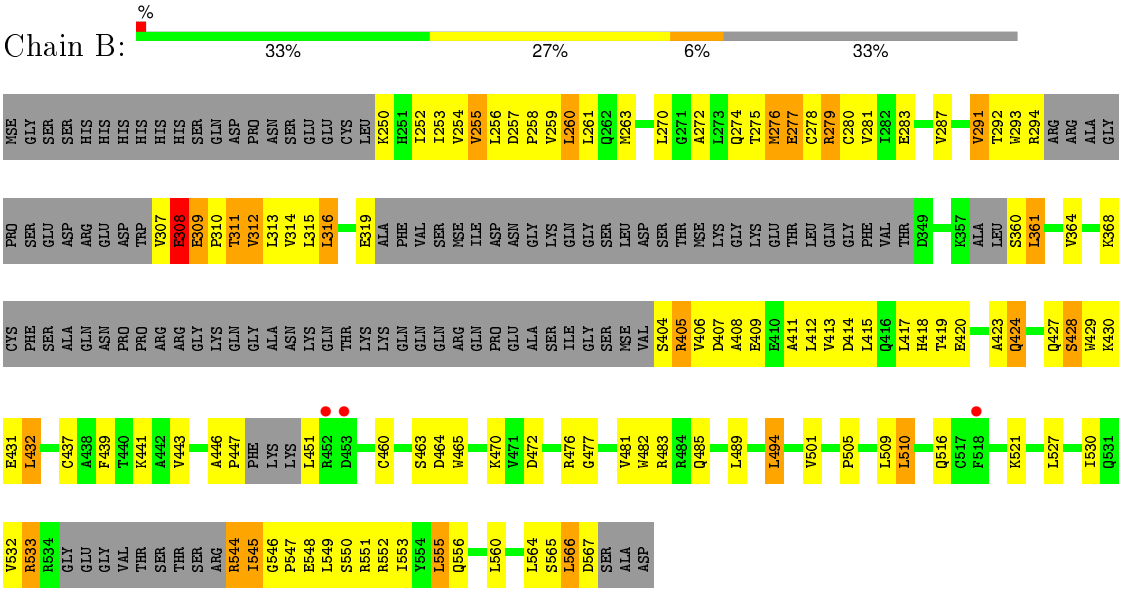
- Molecule 1: Mus81 protein

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	88.96Å 88.96Å 169.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.56 – 2.80 37.56 – 2.71	Depositor EDS
% Data completeness (in resolution range)	95.7 (37.56-2.80) 99.0 (37.56-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [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	999 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.5	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 40839 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.51	0/2184	0.70	0/2934
2	B	0.49	0/1730	0.70	1/2340 (0.0%)
All	All	0.50	0/3914	0.70	1/5274 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	309	GLU	N-CA-C	6.08	127.41	111.00

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	144	0
2	B	1714	0	1663	114	0
All	All	3869	0	3861	249	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 (249) 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:H	2:B:566:LEU:HD12	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
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
2:B:545:ILE:HG23	2:B:549:LEU:HD12	1.62	0.81
1:A:358:ASN:HB2	1:A:521:ASN:ND2	1.94	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: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:HD3	1:A:591:ARG:H	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:N	2:B:544:ARG:HD2	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
1:A:326:ASP:CG	1:A:327:LEU:H	1.92	0.70
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:320:ASP:O	1:A:366:ALA:HA	1.94	0.68
1:A:599:ARG:HH11	1:A:599:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:VAL:O	1:A:539:GLN:HG3	1.94	0.67
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:HB3	2:B:441:LYS:NZ	2.11	0.65
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:426:LEU:HD21	1:A:468:SER:OG	1.96	0.65
1:A:482:LEU:HD13	1:A:510:LEU:HD11	1.77	0.65
1:A:312:TRP:C	1:A:312:TRP:CD1	2.70	0.65
2:B:555:LEU:HD21	2:B:564:LEU:CD2	2.23	0.64
2:B:428:SER:O	2:B:429:TRP:HB2	1.98	0.64
1:A:487:THR:HG23	1:A:488:LEU:N	2.09	0.64
2:B:551:ARG:O	2:B:555:LEU:HB2	1.98	0.64
1:A:531:THR:OG1	1:A:534:GLU:HG3	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
2:B:404:SER:C	2:B:406:VAL:H	2.03	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:549:LEU:HD23	2:B:552:ARG:NH2	2.15	0.61
1:A:481:LYS:O	1:A:482:LEU:CB	2.47	0.61
1:A:514:LEU:HD23	1:A:514:LEU:N	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
2:B:419:THR:HG22	2:B:420:GLU:H	1.69	0.58
1:A:439:ILE:HD12	1:A:439:ILE:N	2.19	0.58
2:B:544:ARG:HG2	2:B:544:ARG:HH11	1.69	0.57
2:B:252:ILE:HG22	2:B:307:VAL:HA	1.87	0.57
1:A:412:LYS:HZ2	1:A:451:THR:HG22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:TYR:O	1:A:481:LYS:O	2.21	0.57
1:A:487:THR:CG2	1:A:488:LEU:H	2.10	0.57
1:A:591:ARG:HG3	1:A:591:ARG:HH21	1.70	0.57
1:A:538:ARG:HD3	2:B:460:CYS:HB2	1.87	0.57
1:A:526:LYS:HB3	1:A:526:LYS:NZ	2.20	0.57
1:A:371:THR:CG2	1:A:372:PRO:HD2	2.31	0.57
2:B:312:VAL:C	2:B:313:LEU:HD12	2.25	0.57
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
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:551:ARG:NH1	2:B:551:ARG:HB3	2.20	0.55
1:A:324:CYS:O	1:A:362:PHE:HA	2.06	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:NH2	1:A:591:ARG:HG3	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
1:A:577:LYS:C	1:A:578:GLU:O	2.45	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:294:ARG:C	2:B:307:VAL:O	2.47	0.52
2:B:472:ASP:OD2	2:B:476:ARG:HB2	2.09	0.52
2:B:275:THR:HG23	2:B:276:MSE:N	2.25	0.52
1:A:326:ASP:CG	1:A:327:LEU:N	2.61	0.52
2:B:258:PRO:HD3	2:B:283:GLU:O	2.09	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
2:B:293:TRP:C	2:B:310:PRO:HD2	2.30	0.51
2:B:311:THR:C	2:B:312:VAL:HG23	2.30	0.51
1:A:368:GLU:OE2	1:A:383:LYS:HG3	2.11	0.51
2:B:293:TRP:O	2:B:310:PRO:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:LYS:HZ3	1:A:526:LYS:HB3	1.76	0.51
2:B:250:LYS:NZ	2:B:276:MSE:SE	2.93	0.51
1:A:578:GLU:C	1:A:580:LEU:H	2.13	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
2:B:257:ASP:O	2:B:260:LEU:HB3	2.11	0.51
1:A:572:SER:O	1:A:573:SER:CB	2.58	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:416:LYS:HG2	1:A:457:PHE:HE1	1.76	0.50
1:A:324:CYS:HB2	1:A:363:LEU:HD23	1.94	0.50
2:B:489:LEU:HD21	2:B:556:GLN:HG2	1.94	0.50
1:A:358:ASN:HB2	1:A:521:ASN:HD21	1.70	0.49
1:A:477:ARG:HH11	1:A:477:ARG:HG3	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
2:B:437:CYS:O	2:B:441:LYS:HG3	2.11	0.49
1:A:607:THR:O	1:A:608:ARG:HB2	2.12	0.49
2:B:252:ILE:O	2:B:252:ILE:HD12	2.12	0.49
1:A:353:ASP:OD2	1:A:355:ARG:NE	2.38	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:483:TYR:O	1:A:485:ASN:N	2.46	0.48
1:A:357:LEU:HD21	1:A:363:LEU:HD22	1.95	0.48
2:B:532:VAL:O	2:B:533:ARG:CB	2.61	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:397:ASP:O	1:A:400:CYS:HB2	2.13	0.48
2:B:544:ARG:O	2:B:545:ILE:CB	2.58	0.48
1:A:557:HIS:CD2	1:A:584:VAL:HG22	2.48	0.48
2:B:494:LEU:HD13	2:B:494:LEU:C	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:HIS:HE1	1:A:315:SER:OG	1.98	0.47
1:A:329:GLU:O	1:A:339:GLN:HG2	2.14	0.47
1:A:363:LEU:HD23	1:A:363:LEU:C	2.36	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
2:B:441:LYS:HB3	2:B:441:LYS:HZ3	1.81	0.45
2:B:404:SER:C	2:B:406:VAL:N	2.70	0.45
1:A:319:TYR:CD1	1:A:319:TYR:C	2.90	0.45
2:B:316:LEU:CD1	2:B:432:LEU:HD11	2.45	0.45
1:A:538:ARG:CD	2:B:460:CYS:HB2	2.46	0.45
2:B:482:TRP:CD1	2:B:501:VAL:HG22	2.52	0.45
1:A:340:GLU:O	1:A:341:LEU:C	2.55	0.44
2:B:420:GLU:N	2:B:420:GLU:OE2	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:HA	1:A:484:GLN:HE21	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
2:B:544:ARG:HG2	2:B:544:ARG:NH1	2.33	0.44
1:A:608:ARG:O	2:B:509:LEU:HG	2.18	0.44
1:A:529:CYS:SG	2:B:565:SER:HB3	2.57	0.44
1:A:481:LYS:HE2	1:A:481:LYS:HB3	1.80	0.44
1:A:314:LEU:C	1:A:314:LEU:HD23	2.39	0.43
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:276:MSE:HE3	2:B:278:CYS:HG	1.83	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:HD22	2:B:560:LEU:N	2.33	0.43
1:A:591:ARG:CD	1:A:591:ARG:H	2.24	0.43
1:A:483:TYR:CD2	1:A:488:LEU:HD11	2.54	0.43
1:A:354:VAL:O	1:A:354:VAL:HG12	2.19	0.43
2:B:428:SER:C	2:B:430:LYS:H	2.22	0.43
2:B:319:GLU:O	2:B:319:GLU:CG	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:SER:O	2:B:361:LEU:CB	2.67	0.43
1:A:357:LEU:HD22	1:A:363:LEU:HD13	2.01	0.43
2:B:552:ARG:HG2	2:B:566:LEU:HB3	2.01	0.42
1:A:513:SER:C	1:A:514:LEU:HD23	2.38	0.42
2:B:254:VAL:HG13	2:B:254:VAL:O	2.19	0.42
2:B:551:ARG:NH1	2:B:567:ASP:O	2.53	0.42
2:B:255:VAL:HA	2:B:281:VAL:O	2.18	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
2:B:250:LYS:O	2:B:250:LYS:HG3	2.20	0.42
1:A:330:THR:O	1:A:330:THR:HG22	2.20	0.42
1:A:390:ILE:HG23	1:A:390:ILE:O	2.20	0.42
2:B:428:SER:OG	2:B:431:GLU:HG3	2.20	0.42
1:A:404:ILE:CG1	1:A:439:ILE:HD11	2.50	0.42
1:A:365:VAL:CG2	1:A:384:GLU:HB3	2.50	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:611:LEU:HD12	2:B:482:TRP:HB2	2.03	0.41
1:A:595:PRO:HG2	1:A:596:ALA:H	1.85	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:CB	2:B:441:LYS:NZ	2.80	0.41
1:A:585:LYS:HD2	1:A:590:LYS:O	2.20	0.41
1:A:359:VAL:HG13	1:A:359:VAL: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
1:A:412:LYS:NZ	1:A:455:ASP:OD2	2.52	0.41
1:A:404:ILE:HG13	1:A:439:ILE:HD11	2.02	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:589:LEU:O	1:A:590:LYS:HB3	2.21	0.40
1:A:462:VAL:CG1	1:A:463:GLN:N	2.83	0.40
1:A:344:GLU:CD	1:A:466:LYS:HE3	2.41	0.40
2:B:510:LEU:HD22	2:B:510:LEU:O	2.21	0.40
2:B:527:LEU:HB3	2:B:530:ILE:HD12	2.03	0.40
2:B:413:VAL:HG12	2:B:417:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:TYR:O	1:A:577:LYS:NZ	2.51	0.40
2:B:446:ALA:HA	2:B:447:PRO:HA	1.89	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%)	2 7
2	B	214/341 (63%)	179 (84%)	23 (11%)	12 (6%)	2 6
All	All	477/652 (73%)	397 (83%)	54 (11%)	26 (6%)	2 6

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
2	B	428	SER

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Mol	Chain	Res	Type
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 (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	241/264 (91%)	217 (90%)	24 (10%)	9 27
2	B	173/282 (61%)	155 (90%)	18 (10%)	9 25
All	All	414/546 (76%)	372 (90%)	42 (10%)	9 27

All (42) 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	341	LEU
1	A	361	ASP
1	A	363	LEU
1	A	371	THR
1	A	412	LYS
1	A	420	LEU
1	A	421	ARG
1	A	425	TYR
1	A	463	GLN
1	A	468	SER

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Mol	Chain	Res	Type
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	255	VAL
2	B	260	LEU
2	B	279	ARG
2	B	291	VAL
2	B	308	GLU
2	B	316	LEU
2	B	407	ASP
2	B	424	GLN
2	B	432	LEU
2	B	463	SER
2	B	470	LYS
2	B	494	LEU
2	B	510	LEU
2	B	516	GLN
2	B	521	LYS
2	B	544	ARG
2	B	555	LEU
2	B	566	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	A	348	ASN
1	A	358	ASN
1	A	446	GLN
1	A	450	ASN
1	A	452	GLN
1	A	484	GLN
1	A	485	ASN
1	A	521	ASN

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Mol	Chain	Res	Type
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	485	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 carbohydrates 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, 95^{th} 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%)	-0.04	5 (1%)	70	59	21, 47, 68, 85	0
2	B	224/341 (65%)	-0.04	3 (1%)	79	71	20, 48, 79, 86	0
All	All	491/652 (75%)	-0.04	8 (1%)	74	66	20, 48, 72, 86	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	430	CYS	3.4
1	A	329	GLU	3.0
1	A	431	GLY	2.7
2	B	453	ASP	2.2
1	A	330	THR	2.2
2	B	452	ARG	2.1
2	B	518	PHE	2.0
1	A	378	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.