Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:48 pm BST

PDB ID	:	4M9R
Title	:	Crystal structure of CED-3
Authors	:	Xu, Y.; Jeffrey, P.D.; Shi, Y.G.
Deposited on	:	2013-08-15
Resolution	:	2.66 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 following versions of software and data (see references ⓘ) were used in the production of this report:

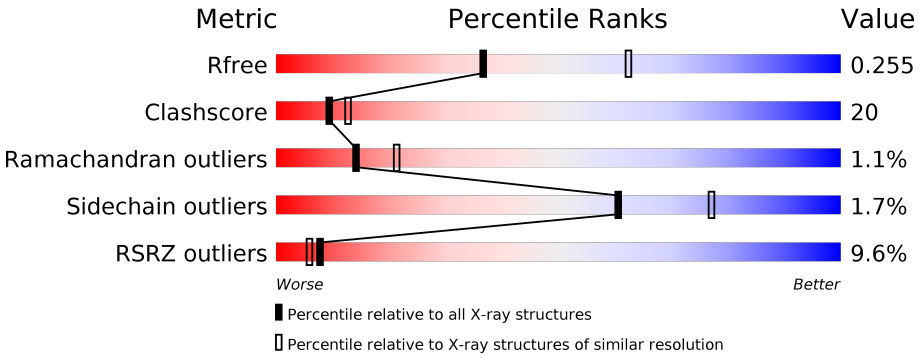
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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	306	8% 51% 31% • 16%
1	B	306	7% 43% 29% • 27%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3821 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 Cell death protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2041	1287	359	381	14			
1	B	223	Total	C	N	O	S	0	0	0
			1773	1123	305	331	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	358	SER	CYS	CONFLICT	UNP P42573
B	358	SER	CYS	CONFLICT	UNP P42573

- Molecule 2 is water.

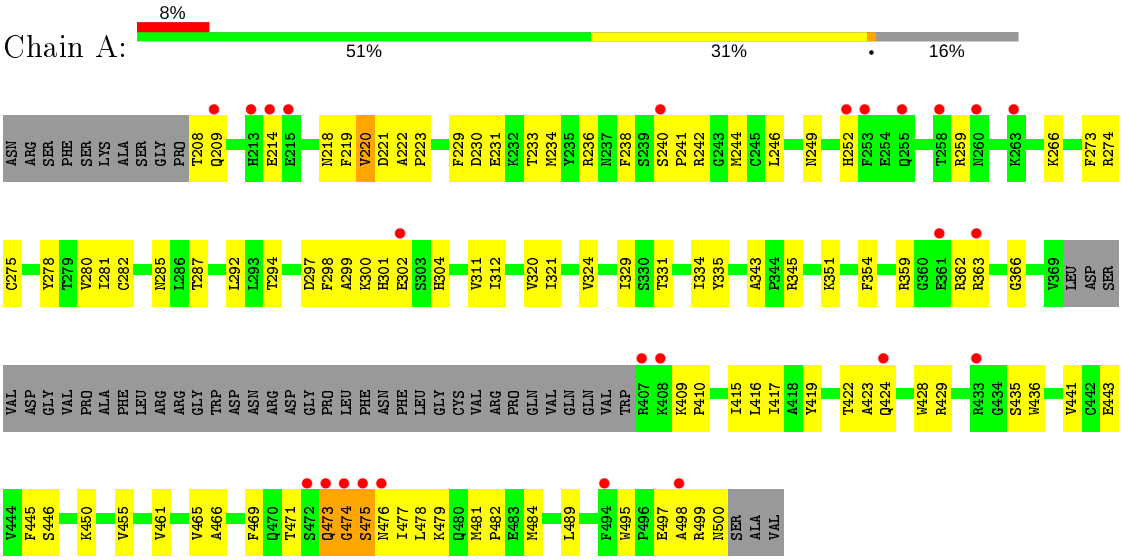
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	5	Total	O	0	0
			5	5		

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 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.

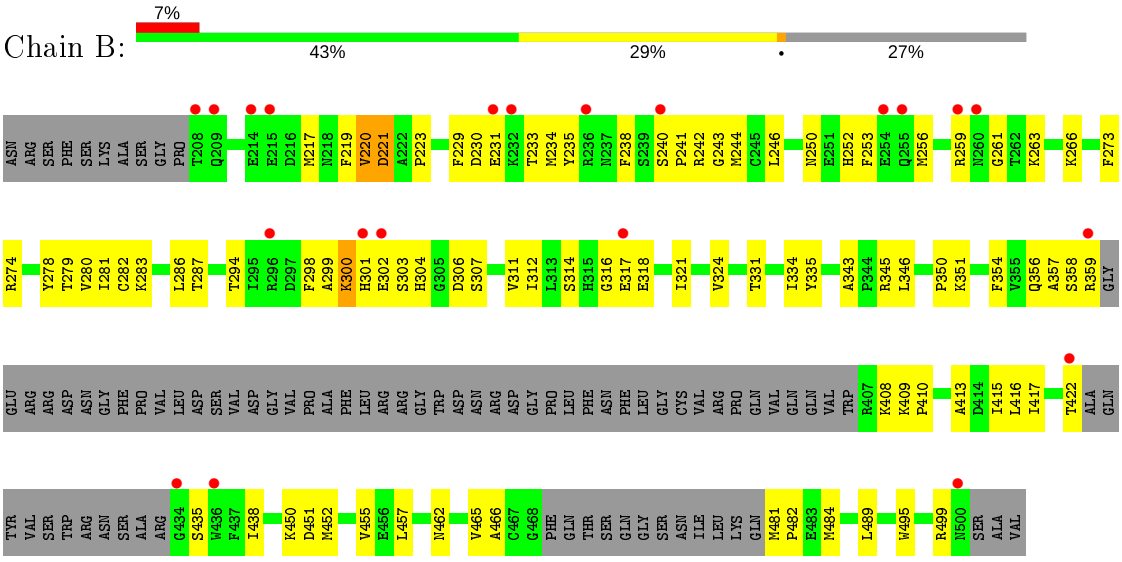
- Molecule 1: Cell death protein 3

Chain A:



- Molecule 1: Cell death protein 3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	121.07Å 121.07Å 58.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.18 – 2.66 20.18 – 2.66	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.18-2.66) 97.2 (20.18-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.206 , 0.260 0.206 , 0.255	Depositor DCC
R_{free} test set	576 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	65.5	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 70.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.037 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3821	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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

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	0.29	0/2083	0.47	0/2814
1	B	0.29	0/1807	0.46	0/2439
All	All	0.29	0/3890	0.46	0/5253

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

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	2041	0	2008	88	0
1	B	1773	0	1751	73	0
2	A	2	0	0	0	0
2	B	5	0	0	0	0
All	All	3821	0	3759	149	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 20.

All (149) 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:465:VAL:HG21	1:A:482:PRO:HG2	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:HG11	1:B:455:VAL:HG11	1.47	0.95
1:A:465:VAL:HG21	1:A:482:PRO:CG	2.02	0.88
1:B:240:SER:O	1:B:499:ARG:HD3	1.85	0.77
1:B:266:LYS:HE2	1:B:282:CYS:SG	2.26	0.75
1:A:423:ALA:O	1:A:424:GLN:HG2	1.87	0.74
1:B:238:PHE:HA	1:B:242:ARG:HH21	1.53	0.72
1:A:351:LYS:HD2	1:A:415:ILE:HG12	1.71	0.72
1:B:252:HIS:O	1:B:324:VAL:HG23	1.90	0.71
1:A:362:ARG:HD3	1:A:424:GLN:HG3	1.70	0.71
1:A:331:THR:O	1:A:334:ILE:HG12	1.91	0.69
1:A:410:PRO:HB2	1:B:481:MET:HB2	1.75	0.68
1:B:316:GLY:O	1:B:359:ARG:HG3	1.93	0.68
1:B:331:THR:O	1:B:334:ILE:HG12	1.94	0.67
1:B:455:VAL:HG13	1:B:484:MET:SD	2.34	0.67
1:B:221:ASP:HB2	1:B:223:PRO:HD2	1.77	0.65
1:B:300:LYS:HA	1:B:345:ARG:HH11	1.60	0.65
1:B:240:SER:HB2	1:B:241:PRO:HD3	1.77	0.65
1:A:477:ILE:HB	1:B:408:LYS:NZ	2.13	0.64
1:A:481:MET:HE2	1:B:410:PRO:HG2	1.79	0.64
1:B:409:LYS:HE2	1:B:489:LEU:HD22	1.79	0.64
1:A:312:ILE:HG21	1:A:321:ILE:HD13	1.79	0.64
1:A:252:HIS:O	1:A:324:VAL:HG23	1.98	0.64
1:B:244:MET:HE3	1:B:279:THR:HB	1.79	0.63
1:A:221:ASP:HB2	1:A:223:PRO:HD2	1.80	0.62
1:A:497:GLU:HG2	1:A:498:ALA:H	1.66	0.61
1:B:230:ASP:HB3	1:B:233:THR:HG22	1.83	0.60
1:B:220:VAL:HG13	1:B:450:LYS:HB2	1.83	0.60
1:B:302:GLU:HG2	1:B:345:ARG:CD	2.31	0.59
1:A:233:THR:HG23	1:A:234:MET:HG2	1.84	0.58
1:B:287:THR:HA	1:B:324:VAL:HG12	1.85	0.58
1:A:287:THR:HA	1:A:324:VAL:HG12	1.86	0.58
1:A:481:MET:CE	1:B:413:ALA:HB2	2.33	0.58
1:B:300:LYS:HG3	1:B:300:LYS:O	2.04	0.57
1:A:479:LYS:HB3	1:B:410:PRO:HG3	1.85	0.57
1:B:273:PHE:O	1:B:278:TYR:HB2	2.06	0.56
1:A:481:MET:HE3	1:B:413:ALA:HB2	1.86	0.56
1:A:455:VAL:HG13	1:A:484:MET:SD	2.45	0.56
1:A:242:ARG:NH2	1:A:499:ARG:NH1	2.55	0.55
1:A:300:LYS:O	1:A:302:GLU:N	2.40	0.54
1:A:240:SER:HB2	1:A:241:PRO:HD3	1.90	0.54
1:A:220:VAL:HG13	1:A:450:LYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:TYR:CG	1:B:350:PRO:HG3	2.43	0.54
1:B:301:HIS:C	1:B:303:SER:H	2.11	0.54
1:A:236:ARG:HG3	1:A:238:PHE:CE2	2.43	0.54
1:A:229:PHE:CE2	1:A:231:GLU:HG3	2.42	0.53
1:A:311:VAL:HG22	1:A:354:PHE:HB2	1.90	0.53
1:A:244:MET:CE	1:A:281:ILE:HD11	2.38	0.53
1:A:436:TRP:CE3	1:A:469:PHE:HB3	2.43	0.53
1:B:311:VAL:HG22	1:B:354:PHE:HB2	1.91	0.53
1:A:240:SER:O	1:A:499:ARG:HD3	2.09	0.53
1:A:359:ARG:O	1:A:424:GLN:HA	2.08	0.53
1:A:249:ASN:HD22	1:A:266:LYS:HD2	1.73	0.52
1:A:474:GLY:O	1:A:475:SER:HB2	2.08	0.52
1:A:266:LYS:CE	1:A:282:CYS:HB3	2.38	0.52
1:B:242:ARG:NH2	1:B:499:ARG:NH1	2.57	0.52
1:A:320:VAL:HA	1:A:329:ILE:O	2.09	0.52
1:B:217:MET:HG2	1:B:219:PHE:CE1	2.45	0.52
1:B:462:ASN:OD1	1:B:482:PRO:HB2	2.10	0.52
1:B:240:SER:HB2	1:B:241:PRO:CD	2.39	0.51
1:A:218:ASN:HB3	1:A:450:LYS:HD3	1.91	0.51
1:A:461:VAL:O	1:A:465:VAL:HG22	2.10	0.51
1:B:253:PHE:HB2	1:B:256:MET:O	2.10	0.51
1:A:455:VAL:HG11	1:B:455:VAL:CG1	2.33	0.51
1:B:246:LEU:HD22	1:B:298:PHE:HB2	1.92	0.51
1:A:455:VAL:CG1	1:B:455:VAL:HG11	2.32	0.50
1:B:274:ARG:HG3	1:B:280:VAL:HG23	1.93	0.50
1:A:473:GLN:HA	1:A:473:GLN:OE1	2.11	0.50
1:A:273:PHE:O	1:A:278:TYR:HB2	2.11	0.50
1:B:283:LYS:HG3	1:B:294:THR:HG21	1.92	0.50
1:B:346:LEU:HB3	1:B:351:LYS:HE3	1.94	0.49
1:B:435:SER:HB2	1:B:438:ILE:HG12	1.94	0.49
1:A:236:ARG:HG3	1:A:238:PHE:HE2	1.77	0.49
1:A:275:CYS:HA	1:A:500:ASN:CB	2.42	0.49
1:B:240:SER:CB	1:B:241:PRO:HD3	2.42	0.49
1:A:298:PHE:O	1:A:304:HIS:HE1	1.96	0.48
1:B:450:LYS:HG3	1:B:451:ASP:N	2.28	0.48
1:B:281:ILE:CD1	1:B:301:HIS:HE1	2.25	0.48
1:A:214:GLU:HG2	1:A:275:CYS:SG	2.52	0.48
1:A:298:PHE:O	1:A:304:HIS:CE1	2.67	0.48
1:A:428:TRP:HZ2	1:A:478:LEU:HD13	1.79	0.48
1:A:335:TYR:HH	1:A:419:TYR:HH	1.60	0.48
1:A:244:MET:HE1	1:A:281:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ALA:HB1	1:B:343:ALA:HB2	1.95	0.47
1:B:302:GLU:HG2	1:B:345:ARG:HD3	1.95	0.47
1:B:250:ASN:O	1:B:259:ARG:HD3	2.15	0.47
1:A:222:ALA:N	1:A:223:PRO:CD	2.78	0.47
1:A:275:CYS:HA	1:A:500:ASN:HB2	1.97	0.47
1:A:422:THR:HG22	1:A:423:ALA:N	2.31	0.46
1:B:302:GLU:C	1:B:304:HIS:H	2.18	0.46
1:A:409:LYS:HE2	1:A:489:LEU:HD22	1.98	0.46
1:B:233:THR:HG23	1:B:234:MET:HG2	1.96	0.46
1:B:465:VAL:HG23	1:B:466:ALA:N	2.31	0.46
1:A:465:VAL:HG21	1:A:482:PRO:CD	2.46	0.46
1:B:306:ASP:O	1:B:350:PRO:HD2	2.17	0.45
1:A:229:PHE:CD1	1:A:238:PHE:HZ	2.34	0.45
1:B:230:ASP:HB3	1:B:233:THR:CG2	2.47	0.45
1:B:317:GLU:HB3	1:B:359:ARG:HD2	1.99	0.45
1:A:416:LEU:C	1:A:416:LEU:HD23	2.37	0.45
1:A:259:ARG:NH1	1:A:429:ARG:NH1	2.65	0.45
1:B:244:MET:HE2	1:B:281:ILE:HD11	2.00	0.44
1:A:429:ARG:HG2	1:A:435:SER:OG	2.17	0.44
1:B:261:GLY:H	1:B:263:LYS:NZ	2.15	0.44
1:B:351:LYS:HD2	1:B:415:ILE:HG12	1.98	0.44
1:A:489:LEU:N	1:A:489:LEU:HD12	2.32	0.44
1:A:297:ASP:O	1:A:300:LYS:HB3	2.18	0.44
1:A:465:VAL:HG23	1:A:466:ALA:N	2.32	0.44
1:B:230:ASP:CB	1:B:233:THR:HG22	2.48	0.44
1:A:443:GLU:O	1:A:446:SER:HB2	2.18	0.44
1:B:465:VAL:HG21	1:B:482:PRO:HG2	1.99	0.44
1:A:266:LYS:HE2	1:A:282:CYS:SG	2.57	0.43
1:A:246:LEU:HD22	1:A:298:PHE:HB2	2.00	0.43
1:A:428:TRP:CZ2	1:A:478:LEU:HD13	2.52	0.43
1:B:229:PHE:CE2	1:B:231:GLU:HG3	2.53	0.43
1:A:238:PHE:HA	1:A:242:ARG:HH21	1.83	0.43
1:A:302:GLU:HG2	1:A:345:ARG:HD3	1.99	0.43
1:A:335:TYR:CZ	1:A:417:ILE:HG12	2.53	0.43
1:A:219:PHE:CD1	1:A:497:GLU:O	2.71	0.43
1:B:298:PHE:HA	1:B:301:HIS:CD2	2.53	0.43
1:B:242:ARG:NH1	1:B:495:TRP:O	2.51	0.43
1:A:274:ARG:HG3	1:A:280:VAL:HG23	2.01	0.43
1:A:441:VAL:O	1:A:445:PHE:HB2	2.18	0.43
1:B:243:GLY:HA3	1:B:307:SER:O	2.19	0.43
1:A:299:ALA:HB1	1:A:343:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLN:O	1:A:474:GLY:C	2.58	0.42
1:B:312:ILE:HG21	1:B:321:ILE:HD13	2.01	0.42
1:A:238:PHE:CE1	1:A:495:TRP:CZ3	3.07	0.42
1:A:230:ASP:CG	1:A:233:THR:HG22	2.39	0.42
1:A:481:MET:HE1	1:B:413:ALA:HB2	2.02	0.42
1:A:246:LEU:HD21	1:A:294:THR:HG22	2.02	0.42
1:A:436:TRP:HZ2	1:A:471:THR:HB	1.84	0.42
1:B:302:GLU:HG2	1:B:345:ARG:NE	2.34	0.42
1:A:417:ILE:HG21	1:A:419:TYR:CZ	2.55	0.41
1:B:240:SER:CB	1:B:241:PRO:CD	2.99	0.41
1:A:240:SER:HB2	1:A:241:PRO:CD	2.49	0.41
1:B:358:SER:HA	1:B:422:THR:HB	2.03	0.41
1:A:208:THR:C	1:A:209:GLN:HG3	2.41	0.41
1:A:230:ASP:OD2	1:A:233:THR:HG22	2.21	0.41
1:A:366:GLY:HA2	1:B:409:LYS:O	2.21	0.41
1:B:416:LEU:HD23	1:B:416:LEU:C	2.41	0.41
1:A:363:ARG:HB3	1:A:478:LEU:HD22	2.02	0.41
1:B:335:TYR:CZ	1:B:417:ILE:HG12	2.55	0.41
1:B:314:SER:O	1:B:357:ALA:HA	2.21	0.41
1:B:283:LYS:HB3	1:B:286:LEU:HD11	2.02	0.41
1:A:244:MET:HE2	1:A:281:ILE:HD11	2.02	0.40
1:A:230:ASP:HB3	1:A:233:THR:HG22	2.03	0.40
1:B:452:MET:HB2	1:B:457:LEU:CD2	2.52	0.40
1:A:292:LEU:HD21	1:A:329:ILE:HG23	2.03	0.40
1:A:466:ALA:HB1	1:B:410:PRO:HD2	2.04	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	252/306 (82%)	230 (91%)	18 (7%)	4 (2%)	9 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	215/306 (70%)	199 (93%)	15 (7%)	1 (0%)	29 43
All	All	467/612 (76%)	429 (92%)	33 (7%)	5 (1%)	14 21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	HIS
1	A	474	GLY
1	A	475	SER
1	A	285	ASN
1	B	318	GLU

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	224/267 (84%)	221 (99%)	3 (1%)	69 82
1	B	196/267 (73%)	192 (98%)	4 (2%)	55 73
All	All	420/534 (79%)	413 (98%)	7 (2%)	60 77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	VAL
1	A	473	GLN
1	A	476	ASN
1	B	220	VAL
1	B	221	ASP
1	B	300	LYS
1	B	356	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	304	HIS
1	A	356	GLN
1	A	500	ASN
1	B	301	HIS

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	256/306 (83%)	0.45	25 (9%)	7 5	44, 76, 137, 183	0
1	B	223/306 (72%)	0.36	21 (9%)	8 6	44, 75, 140, 186	0
All	All	479/612 (78%)	0.41	46 (9%)	8 6	44, 76, 140, 186	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	ARG	6.5
1	A	408	LYS	6.2
1	A	258	THR	5.5
1	A	252	HIS	5.4
1	B	209	GLN	5.2
1	B	260	ASN	5.0
1	B	359	ARG	4.7
1	A	361	GLU	4.6
1	B	208	THR	4.3
1	A	253	PHE	4.2
1	B	240	SER	4.2
1	B	255	GLN	4.1
1	B	231	GLU	4.1
1	B	436	TRP	4.0
1	A	209	GLN	4.0
1	B	302	GLU	3.9
1	A	475	SER	3.8
1	A	263	LYS	3.8
1	B	317	GLU	3.7
1	A	363	ARG	3.7
1	B	215	GLU	3.6
1	A	433	ARG	3.3
1	A	472	SER	3.2
1	A	260	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	254	GLU	2.9
1	B	232	LYS	2.9
1	A	498	ALA	2.9
1	B	301	HIS	2.9
1	B	434	GLY	2.7
1	A	476	ASN	2.7
1	A	255	GLN	2.7
1	B	500	ASN	2.7
1	B	214	GLU	2.6
1	B	236	ARG	2.5
1	B	296	ARG	2.5
1	A	302	GLU	2.5
1	A	473	GLN	2.4
1	B	422	THR	2.4
1	A	240	SER	2.3
1	B	259	ARG	2.3
1	A	494	PHE	2.2
1	A	215	GLU	2.2
1	A	474	GLY	2.1
1	A	424	GLN	2.1
1	A	213	HIS	2.0
1	A	214	GLU	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

There are no such residues in this entry.