Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:16 AM GMT

PDB ID	:	3E1S
Title	:	Structure of an N-terminal truncation of Deinococcus radiodurans RecD2
Authors	:	Saikrishnan, K.; Griffiths, S.P.; Cook, N.; Court, R.; Wigley, D.B.
Deposited on	:	2008-08-04
Resolution	:	2.20 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:

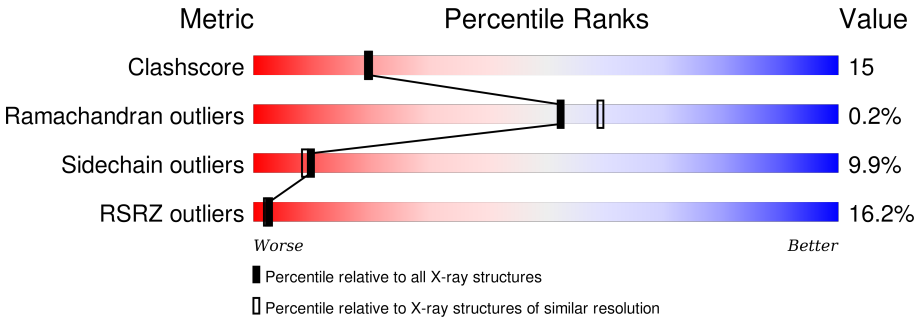
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	574	15% 64% 23% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4154 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 Exodeoxyribonuclease V, subunit RecD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			3889	2443	717	719	10			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	MET	-	EXPRESSION TAG	UNP Q9RT63
A	716	LEU	-	EXPRESSION TAG	UNP Q9RT63
A	717	GLU	-	EXPRESSION TAG	UNP Q9RT63
A	718	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	719	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	720	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	721	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	722	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	723	HIS	-	EXPRESSION TAG	UNP Q9RT63

- Molecule 2 is water.

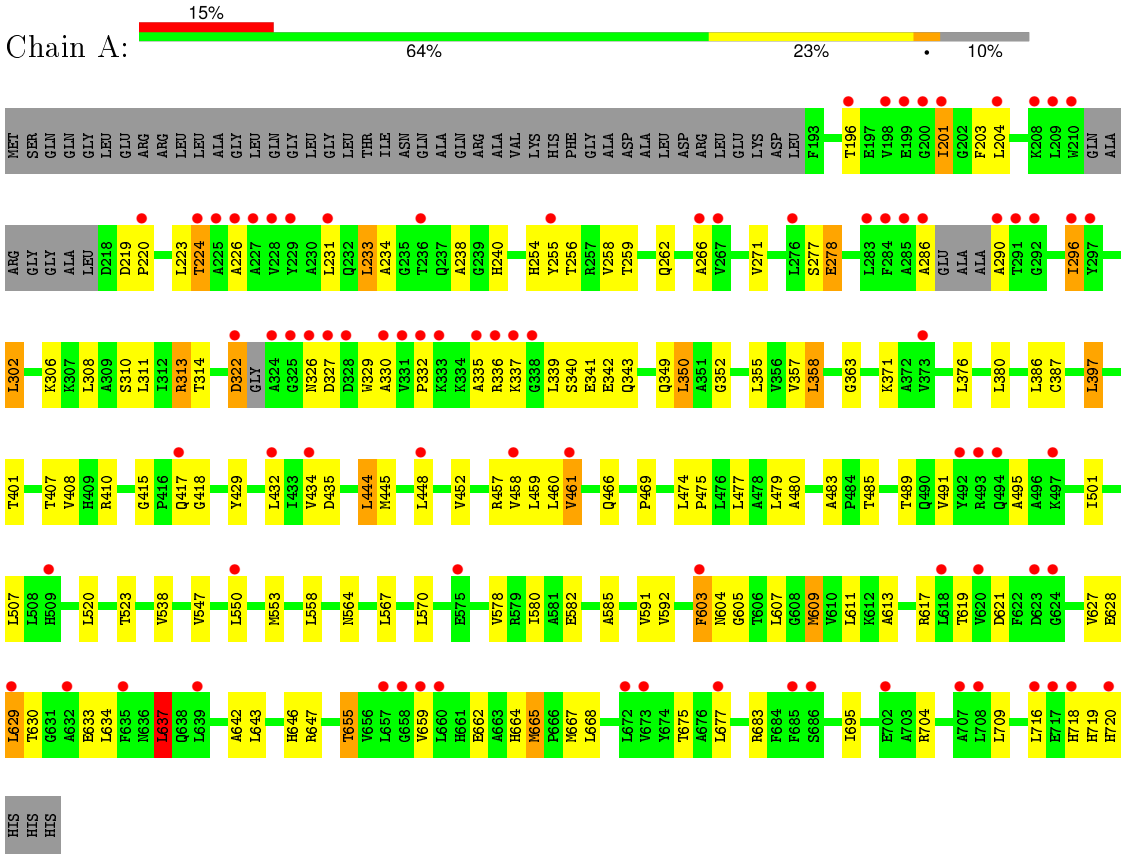
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	265	Total	O	0	0
			265	265		

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: Exodeoxyribonuclease V, subunit RecD

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.63Å 89.63Å 131.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.70 – 2.20 19.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.70-2.20) 98.2 (19.96-2.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.231 , 0.287 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 32947 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4154	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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	0.46	0/3962	0.67	3/5382 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	605	GLY	O-C-N	-5.98	113.13	122.70
1	A	637	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	352	GLY	O-C-N	-5.12	114.52	122.70

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	3889	0	3920	116	0
2	A	265	0	0	9	0
All	All	4154	0	3920	116	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 15.

All (116) 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:665:MET:CE	1:A:668:LEU:HD12	1.83	1.08
1:A:480:ALA:HA	1:A:485:THR:HG21	1.56	0.86
1:A:665:MET:HE3	1:A:668:LEU:HD12	1.55	0.85
1:A:220:PRO:O	1:A:224:THR:HG23	1.77	0.84
1:A:340:SER:H	1:A:343:GLN:HE21	1.28	0.82
1:A:665:MET:HE1	1:A:695:ILE:HG21	1.61	0.81
1:A:553:MET:HE3	1:A:664:HIS:HA	1.62	0.81
1:A:564:ASN:HD21	1:A:642:ALA:H	1.30	0.80
1:A:619:THR:HG22	1:A:628:GLU:HG2	1.65	0.79
1:A:603:PHE:HD1	1:A:604:ASN:H	1.31	0.79
1:A:558:LEU:HB3	1:A:659:VAL:HG11	1.65	0.78
1:A:417:GLN:HB2	2:A:798:HOH:O	1.86	0.76
1:A:592:VAL:HG22	1:A:607:LEU:HD23	1.68	0.76
1:A:483:ALA:O	1:A:485:THR:HG23	1.86	0.75
1:A:417:GLN:NE2	1:A:418:GLY:O	2.20	0.74
1:A:553:MET:HE3	1:A:664:HIS:CA	2.19	0.72
1:A:387:CYS:SG	1:A:408:VAL:HA	2.33	0.69
1:A:417:GLN:CB	2:A:798:HOH:O	2.41	0.68
1:A:226:ALA:HB1	1:A:256:THR:HG21	1.73	0.68
1:A:665:MET:HE1	1:A:668:LEU:HD12	1.74	0.68
1:A:259:THR:H	1:A:262:GLN:HE21	1.42	0.68
1:A:452:VAL:HG21	1:A:458:VAL:HG21	1.77	0.67
1:A:329:TRP:HA	1:A:380:LEU:HD13	1.77	0.67
1:A:233:LEU:HD23	1:A:255:TYR:CZ	2.30	0.67
1:A:271:VAL:HG11	1:A:278:GLU:CG	2.25	0.66
1:A:226:ALA:CB	1:A:256:THR:HG21	2.25	0.66
1:A:523:THR:HG23	2:A:790:HOH:O	1.96	0.65
1:A:578:VAL:HG23	1:A:613:ALA:HB1	1.77	0.64
1:A:609:MET:O	1:A:611:LEU:HD22	1.97	0.64
1:A:313:ARG:HE	1:A:314:THR:HG22	1.63	0.64
1:A:271:VAL:HG11	1:A:278:GLU:HG3	1.81	0.63
1:A:337:LYS:HE3	2:A:882:HOH:O	1.99	0.62
1:A:564:ASN:ND2	1:A:642:ALA:H	1.98	0.62
1:A:310:SER:O	1:A:314:THR:HG23	2.01	0.61
1:A:434:VAL:HG21	1:A:448:LEU:HD21	1.83	0.60
1:A:417:GLN:HA	2:A:798:HOH:O	2.00	0.60
1:A:553:MET:HE1	1:A:667:MET:HG2	1.82	0.60
1:A:302:LEU:HD22	1:A:306:LYS:HD2	1.82	0.59
1:A:350:LEU:O	1:A:457:ARG:NH1	2.35	0.59
1:A:665:MET:HA	1:A:665:MET:CE	2.32	0.59
1:A:469:PRO:O	1:A:704:ARG:NH2	2.34	0.59
1:A:655:THR:HG22	2:A:727:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:VAL:HB	1:A:485:THR:HG22	1.85	0.58
1:A:386:LEU:HD23	1:A:397:LEU:HD22	1.86	0.57
1:A:204:LEU:HD12	1:A:204:LEU:H	1.68	0.57
1:A:342:GLU:OE2	1:A:489:THR:HG22	2.04	0.57
1:A:655:THR:HG21	1:A:683:ARG:HH21	1.71	0.55
1:A:387:CYS:SG	1:A:408:VAL:HG22	2.47	0.55
1:A:271:VAL:CG1	1:A:278:GLU:HG3	2.36	0.54
1:A:417:GLN:CA	2:A:798:HOH:O	2.56	0.54
1:A:538:VAL:HG13	1:A:547:VAL:CG1	2.37	0.54
1:A:627:VAL:HG22	1:A:629:LEU:HD13	1.90	0.53
1:A:655:THR:HB	1:A:683:ARG:HB2	1.91	0.53
1:A:408:VAL:HG11	1:A:444:LEU:HD12	1.90	0.53
1:A:603:PHE:HD1	1:A:604:ASN:N	2.04	0.52
1:A:434:VAL:HG21	1:A:448:LEU:CD2	2.40	0.52
1:A:665:MET:HA	1:A:665:MET:HE2	1.92	0.52
1:A:665:MET:HE3	1:A:668:LEU:CD1	2.35	0.52
1:A:407:THR:HG23	1:A:410:ARG:HH11	1.75	0.52
1:A:271:VAL:HG21	1:A:278:GLU:HG2	1.91	0.52
1:A:495:ALA:HB1	1:A:501:ILE:HD12	1.91	0.51
1:A:336:ARG:HA	1:A:339:LEU:HD22	1.92	0.51
1:A:591:VAL:HG11	1:A:637:LEU:HG	1.92	0.51
1:A:627:VAL:HG22	1:A:629:LEU:CD1	2.42	0.50
1:A:371:LYS:HG3	1:A:401:THR:HA	1.93	0.49
1:A:363:GLY:HA3	1:A:491:VAL:HG13	1.94	0.49
1:A:630:THR:CA	1:A:634:LEU:HD13	2.42	0.49
1:A:480:ALA:CA	1:A:485:THR:HG21	2.35	0.49
1:A:630:THR:HA	1:A:634:LEU:HD13	1.95	0.49
1:A:231:LEU:O	1:A:234:ALA:HB3	2.12	0.49
1:A:329:TRP:CZ2	1:A:376:LEU:HD12	2.47	0.49
1:A:322:ASP:N	1:A:326:ASN:OD1	2.41	0.48
1:A:223:LEU:CD2	1:A:258:VAL:HG11	2.43	0.48
1:A:592:VAL:HG22	1:A:607:LEU:CD2	2.41	0.48
1:A:553:MET:HE1	1:A:667:MET:CG	2.44	0.48
1:A:231:LEU:HD21	1:A:296:ILE:HD11	1.94	0.47
1:A:259:THR:HG23	1:A:262:GLN:NE2	2.29	0.47
1:A:507:LEU:HD11	1:A:677:LEU:HD22	1.94	0.47
1:A:286:ALA:O	1:A:290:ALA:N	2.48	0.47
1:A:226:ALA:HB1	1:A:256:THR:CG2	2.41	0.47
1:A:201:ILE:H	1:A:201:ILE:HD12	1.81	0.45
1:A:655:THR:CG2	2:A:727:HOH:O	2.61	0.45
1:A:452:VAL:HG21	1:A:458:VAL:CG2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ARG:HE	1:A:628:GLU:HB3	1.82	0.45
1:A:415:GLY:N	1:A:417:GLN:HE22	2.13	0.45
1:A:434:VAL:O	1:A:461:VAL:HG13	2.17	0.44
1:A:466:GLN:HE22	1:A:675:THR:HA	1.82	0.44
1:A:466:GLN:NE2	1:A:675:THR:OG1	2.51	0.44
1:A:580:ILE:HD13	1:A:585:ALA:HB2	2.00	0.44
1:A:271:VAL:HG11	1:A:278:GLU:CD	2.38	0.43
1:A:233:LEU:HD23	1:A:255:TYR:CE1	2.54	0.43
1:A:435:ASP:OD2	1:A:461:VAL:HG22	2.19	0.43
1:A:474:LEU:HD22	1:A:477:LEU:HD22	2.00	0.43
1:A:277:SER:O	1:A:296:ILE:HA	2.19	0.43
1:A:196:THR:HG23	1:A:203:PHE:HB2	2.01	0.43
1:A:223:LEU:HD23	1:A:258:VAL:HG11	2.01	0.42
1:A:408:VAL:HG11	1:A:444:LEU:CD1	2.49	0.42
1:A:326:ASN:ND2	1:A:327:ASP:O	2.53	0.42
1:A:220:PRO:HA	1:A:223:LEU:HD12	2.02	0.42
1:A:611:LEU:HD21	1:A:621:ASP:HB2	2.01	0.42
1:A:460:LEU:CD1	1:A:479:LEU:HD13	2.50	0.42
1:A:313:ARG:NE	1:A:314:THR:HG22	2.31	0.42
1:A:233:LEU:HD23	1:A:255:TYR:CE2	2.54	0.42
1:A:223:LEU:HB3	1:A:266:ALA:HB2	2.01	0.42
1:A:474:LEU:N	1:A:475:PRO:HD3	2.35	0.41
1:A:538:VAL:HG13	1:A:547:VAL:HG13	2.02	0.41
1:A:238:ALA:HB3	1:A:240:HIS:CD2	2.55	0.41
1:A:611:LEU:HD21	1:A:621:ASP:CB	2.50	0.41
1:A:429:TYR:CD2	1:A:432:LEU:HD21	2.54	0.41
1:A:550:LEU:HA	1:A:643:LEU:O	2.21	0.41
1:A:358:LEU:O	1:A:461:VAL:HA	2.21	0.41
1:A:452:VAL:CG2	1:A:458:VAL:HG21	2.47	0.41
1:A:591:VAL:CG1	1:A:637:LEU:HG	2.51	0.41
1:A:332:PRO:HG2	1:A:335:ALA:HB2	2.02	0.41
1:A:330:ALA:O	1:A:376:LEU:HD21	2.21	0.41
1:A:646:HIS:HE1	2:A:783:HOH:O	2.04	0.41

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	509/574 (89%)	491 (96%)	17 (3%)	1 (0%)	52 59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	662	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	393/435 (90%)	354 (90%)	39 (10%)	10 9

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	ILE
1	A	219	ASP
1	A	224	THR
1	A	233	LEU
1	A	254	HIS
1	A	278	GLU
1	A	296	ILE
1	A	302	LEU
1	A	308	LEU
1	A	311	LEU

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Mol	Chain	Res	Type
1	A	313	ARG
1	A	322	ASP
1	A	341	GLU
1	A	349	GLN
1	A	350	LEU
1	A	355	LEU
1	A	358	LEU
1	A	397	LEU
1	A	444	LEU
1	A	445	MET
1	A	459	LEU
1	A	461	VAL
1	A	520	LEU
1	A	567	LEU
1	A	570	LEU
1	A	582	GLU
1	A	603	PHE
1	A	609	MET
1	A	629	LEU
1	A	633	GLU
1	A	637	LEU
1	A	647	ARG
1	A	655	THR
1	A	665	MET
1	A	709	LEU
1	A	716	LEU
1	A	718	HIS
1	A	719	HIS
1	A	720	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	GLN
1	A	343	GLN
1	A	466	GLN
1	A	481	GLN
1	A	490	GLN
1	A	502	GLN
1	A	564	ASN
1	A	566	HIS
1	A	568	GLN

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Mol	Chain	Res	Type
1	A	572	ASN
1	A	593	GLN
1	A	625	ASN
1	A	646	HIS
1	A	664	HIS
1	A	671	ASN

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	517/574 (90%)	0.90	84 (16%)	3 2	49, 54, 62, 76	2 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	GLU	5.9
1	A	322	ASP	5.6
1	A	327	ASP	5.6
1	A	204	LEU	5.5
1	A	624	GLY	5.5
1	A	227	ALA	5.3
1	A	331	VAL	5.2
1	A	324	ALA	5.0
1	A	325	GLY	4.7
1	A	226	ALA	4.7
1	A	338	GLY	4.5
1	A	210	TRP	4.5
1	A	290	ALA	4.5
1	A	657	LEU	4.4
1	A	720	HIS	4.3
1	A	228	VAL	4.2
1	A	199	GLU	3.9
1	A	718	HIS	3.9
1	A	225	ALA	3.8
1	A	285	ALA	3.8
1	A	659	VAL	3.7
1	A	255	TYR	3.7
1	A	208	LYS	3.7
1	A	417	GLN	3.6
1	A	336	ARG	3.5
1	A	337	LYS	3.5
1	A	201	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	326	ASN	3.4
1	A	702	GLU	3.4
1	A	296	ILE	3.4
1	A	198	VAL	3.3
1	A	635	PHE	3.3
1	A	632	ALA	3.2
1	A	658	GLY	3.1
1	A	639	LEU	3.1
1	A	229	TYR	3.1
1	A	708	LEU	3.1
1	A	434	VAL	3.1
1	A	209	LEU	3.1
1	A	494	GLN	3.1
1	A	284	PHE	3.0
1	A	328	ASP	3.0
1	A	291	THR	3.0
1	A	267	VAL	3.0
1	A	333	LYS	2.9
1	A	492	TYR	2.9
1	A	335	ALA	2.8
1	A	707	ALA	2.8
1	A	677	LEU	2.8
1	A	493	ARG	2.7
1	A	620	VAL	2.7
1	A	673	VAL	2.6
1	A	497	LYS	2.6
1	A	196	THR	2.6
1	A	686	SER	2.5
1	A	292	GLY	2.5
1	A	603	PHE	2.5
1	A	716	LEU	2.5
1	A	266	ALA	2.4
1	A	297	TYR	2.4
1	A	276	LEU	2.4
1	A	458	VAL	2.4
1	A	623	ASP	2.4
1	A	283	LEU	2.3
1	A	685	PHE	2.3
1	A	550	LEU	2.3
1	A	618	LEU	2.3
1	A	629	LEU	2.3
1	A	373	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	231	LEU	2.3
1	A	332	PRO	2.3
1	A	236	THR	2.2
1	A	448	LEU	2.2
1	A	224	THR	2.2
1	A	330	ALA	2.2
1	A	220	PRO	2.2
1	A	660	LEU	2.2
1	A	432	LEU	2.1
1	A	509	HIS	2.1
1	A	461	VAL	2.1
1	A	575	GLU	2.1
1	A	672	LEU	2.0
1	A	286	ALA	2.0
1	A	200	GLY	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 carbohydrates 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.