Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:51 PM GMT

PDB ID	:	4DNV
Title	:	Crystal structure of the W285F mutant of UVB-resistance protein UVR8
Authors	:	Wu, D.; Hu, Q.; Yan, Z.; Chen, W.; Yan, C.; Zhang, J.; Wang, J.; Shi, Y.
Deposited on	:	2012-02-09
Resolution	:	2.00 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:

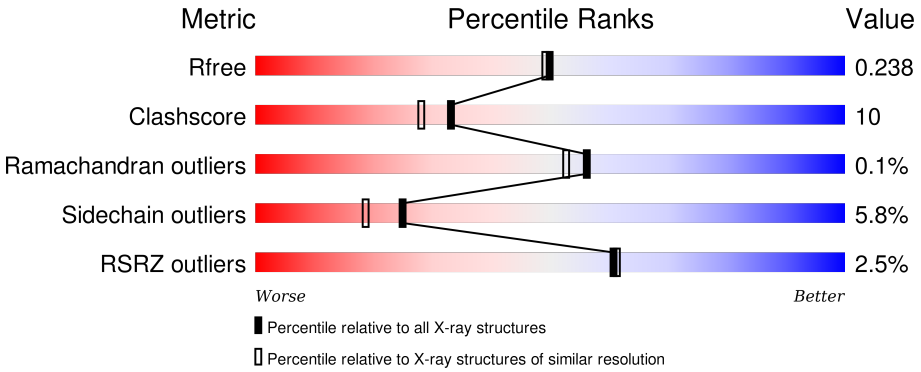
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	370	2% 83% 15%
1	B	370	2% 75% 22%
1	C	370	2% 74% 24%
1	D	370	4% 78% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11846 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 AT5g63860/MGI19_6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2802	1747	506	536	13			
1	B	368	Total	C	N	O	S	0	0	0
			2786	1736	503	534	13			
1	C	370	Total	C	N	O	S	0	1	0
			2810	1752	507	537	14			
1	D	368	Total	C	N	O	S	0	0	0
			2790	1739	504	534	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	PHE	TRP	ENGINEERED MUTATION	UNP Q9FN03
B	285	PHE	TRP	ENGINEERED MUTATION	UNP Q9FN03
C	285	PHE	TRP	ENGINEERED MUTATION	UNP Q9FN03
D	285	PHE	TRP	ENGINEERED MUTATION	UNP Q9FN03

- Molecule 2 is water.

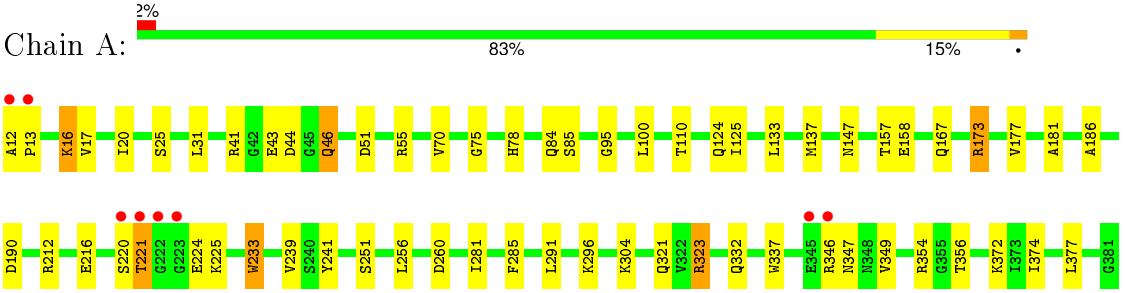
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	176	Total	O	0	0
			176	176		
2	B	166	Total	O	0	0
			166	166		
2	C	171	Total	O	0	0
			171	171		
2	D	145	Total	O	0	0
			145	145		

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.

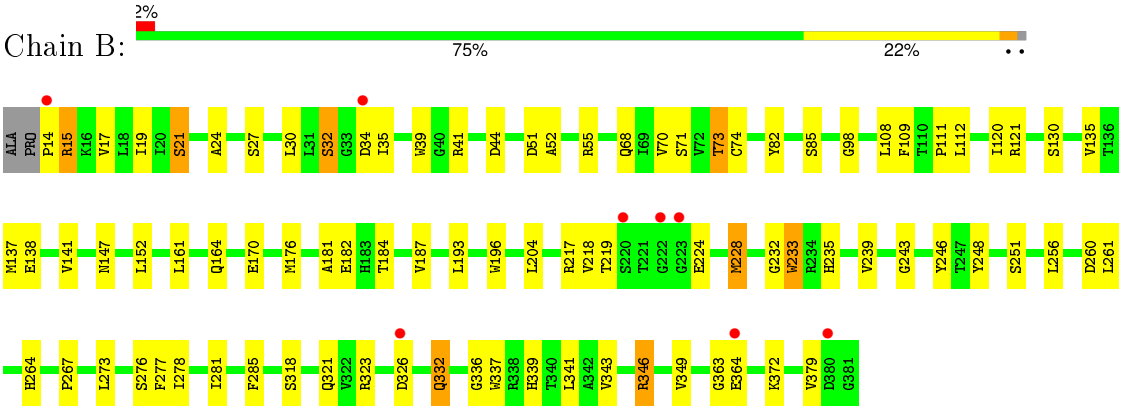
- Molecule 1: AT5g63860/MGI19_6

Chain A:



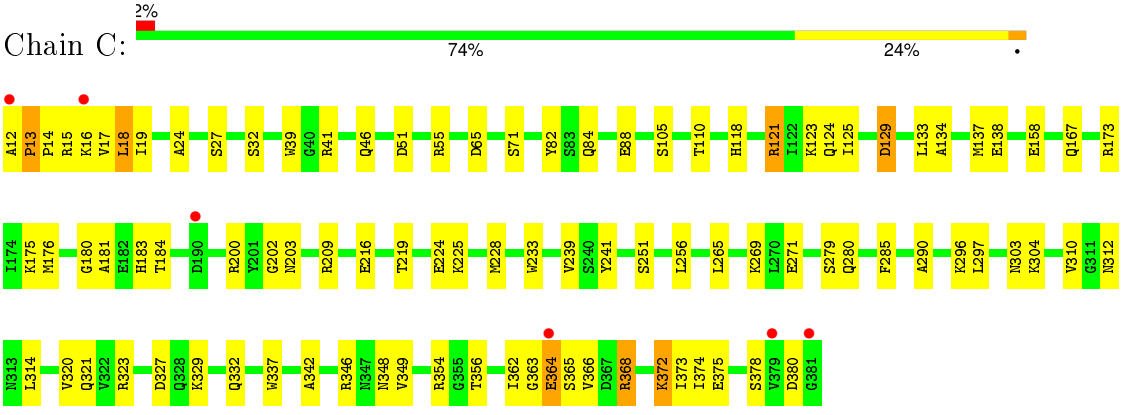
- Molecule 1: AT5g63860/MGI19_6

Chain B:



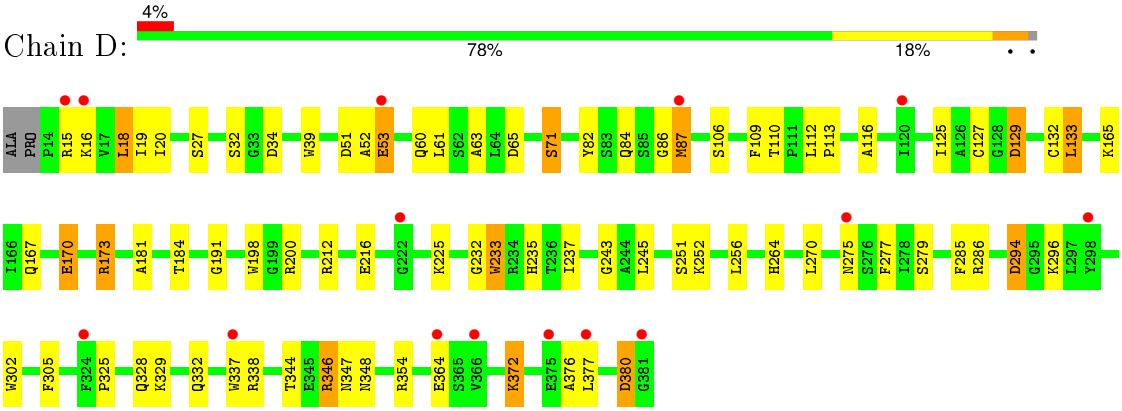
- Molecule 1: AT5g63860/MGI19_6

Chain C:



• Molecule 1: AT5g63860/MGI19_6

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.57Å 67.21Å 93.63Å 85.06° 81.45° 66.04°	Depositor
Resolution (Å)	33.02 – 2.00 33.02 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (33.02-2.00) 92.9 (33.02-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.207 , 0.240 0.205 , 0.238	Depositor DCC
R_{free} test set	3875 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.0	EDS
Estimated twinning fraction	0.015 for -h,-h+k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 77452 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11846	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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	0.45	0/2869	0.56	0/3890
1	B	0.43	0/2852	0.57	1/3866 (0.0%)
1	C	0.43	0/2877	0.56	0/3900
1	D	0.41	0/2856	0.54	0/3870
All	All	0.43	0/11454	0.56	1/15526 (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})
1	B	193	LEU	CA-CB-CG	5.06	126.94	115.30

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	2802	0	2680	51	1
1	B	2786	0	2658	62	1
1	C	2810	0	2688	57	1
1	D	2790	0	2669	62	1
2	A	176	0	0	8	0
2	B	166	0	0	12	0
2	C	171	0	0	4	0
2	D	145	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11846	0	10695	226	2

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 10.

All (226) 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:B:138:GLU:HG3	2:B:564:HOH:O	1.36	1.24
1:D:51:ASP:OD2	1:D:53:GLU:HG3	1.66	0.93
1:B:248:TYR:HB2	2:B:532:HOH:O	1.66	0.93
1:D:170:GLU:HG3	2:D:524:HOH:O	1.73	0.89
1:C:65:ASP:OD2	2:C:541:HOH:O	1.90	0.89
1:B:264:HIS:O	2:B:532:HOH:O	1.92	0.86
1:C:375:GLU:OE2	1:C:375:GLU:HA	1.77	0.84
1:D:20:ILE:O	1:D:20:ILE:HD12	1.77	0.84
1:A:137:MET:HE3	1:A:137:MET:HA	1.60	0.84
1:A:46:GLN:HE21	1:A:46:GLN:H	1.22	0.83
1:A:285:PHE:HB2	1:A:337:TRP:HA	1.62	0.80
1:B:14:PRO:HG2	1:B:379:VAL:HA	1.62	0.80
1:D:84:GLN:O	2:D:471:HOH:O	2.01	0.79
1:A:220:SER:O	1:A:221:THR:HB	1.81	0.78
1:D:18:LEU:N	1:D:18:LEU:HD13	1.98	0.78
1:A:221:THR:O	1:A:221:THR:HG23	1.86	0.75
1:B:19:ILE:HD12	1:B:71:SER:HA	1.67	0.75
1:C:279:SER:O	1:C:280:GLN:NE2	2.17	0.74
1:A:44:ASP:H	1:A:46:GLN:HE22	1.34	0.74
1:A:260:ASP:OD1	2:A:421:HOH:O	2.05	0.74
1:D:191:GLY:HA3	1:D:225:LYS:HB3	1.69	0.74
1:A:220:SER:O	1:A:221:THR:CB	2.36	0.73
1:A:181:ALA:HB2	1:A:233:TRP:CD1	2.23	0.73
1:A:70:VAL:HG21	1:A:84:GLN:HG3	1.72	0.72
1:C:15:ARG:HD3	1:C:32:SER:O	1.89	0.72
1:B:339:HIS:ND1	2:B:407:HOH:O	2.13	0.71
1:D:86:GLY:C	1:D:87:MET:HG2	2.10	0.71
1:B:321:GLN:HE22	1:B:323:ARG:NH1	1.90	0.70
1:B:260:ASP:O	1:B:261:LEU:HD23	1.93	0.69
1:D:19:ILE:HA	1:D:332:GLN:HE22	1.58	0.68
1:B:181:ALA:HB2	1:B:233:TRP:CD1	2.29	0.68
1:A:17:VAL:HG11	1:A:20:ILE:HG23	1.74	0.68
1:A:167:GLN:HB2	2:A:552:HOH:O	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ALA:HA	1:B:337:TRP:CD1	2.30	0.67
1:C:200:ARG:O	1:C:209:ARG:HD3	1.95	0.67
1:D:294:ASP:O	1:D:329:LYS:HD3	1.93	0.67
1:B:228:MET:HG3	1:B:239:VAL:HB	1.77	0.67
1:B:27:SER:HB3	1:B:341:LEU:HD11	1.75	0.67
1:C:304:LYS:HE2	1:D:109:PHE:CE2	2.31	0.66
1:D:325:PRO:O	1:D:328:GLN:HG2	1.96	0.66
1:D:18:LEU:N	1:D:18:LEU:CD1	2.60	0.65
1:C:323:ARG:NH1	1:C:327:ASP:OD1	2.26	0.65
1:B:170:GLU:O	2:B:482:HOH:O	2.13	0.65
1:B:285:PHE:HB2	1:B:337:TRP:HA	1.80	0.64
1:D:16:LYS:N	1:D:32:SER:OG	2.31	0.64
1:A:46:GLN:NE2	1:A:46:GLN:H	1.93	0.64
1:C:24:ALA:HA	1:C:337:TRP:CD1	2.32	0.64
1:C:51:ASP:OD1	1:C:55:ARG:NH2	2.30	0.63
1:A:304:LYS:HE2	1:B:109:PHE:CZ	2.34	0.62
1:C:285:PHE:HB2	1:C:337:TRP:HA	1.81	0.62
1:A:16:LYS:HE3	1:A:347:ASN:OD1	1.99	0.62
1:C:296:LYS:HG2	1:C:321:GLN:OE1	2.00	0.61
1:A:124:GLN:HG2	1:A:125:ILE:N	2.17	0.60
1:D:346:ARG:NH2	1:D:380:ASP:OD1	2.35	0.60
1:B:71:SER:HB3	1:B:82:TYR:CE2	2.37	0.59
1:D:165:LYS:HD3	1:D:167:GLN:NE2	2.17	0.59
1:C:375:GLU:HG2	2:C:480:HOH:O	2.02	0.59
1:B:273:LEU:O	2:B:456:HOH:O	2.17	0.59
1:B:164:GLN:NE2	2:B:516:HOH:O	2.36	0.59
1:B:218:VAL:HG11	1:B:267:PRO:HG2	1.86	0.58
1:B:121:ARG:HB3	1:B:137:MET:CG	2.34	0.58
1:A:51:ASP:OD1	1:A:55:ARG:NH2	2.37	0.58
1:C:124:GLN:HG2	1:C:125:ILE:N	2.19	0.58
1:B:135:VAL:HG22	1:B:141:VAL:HG22	1.84	0.58
1:B:121:ARG:HD2	1:B:137:MET:HG3	1.86	0.57
1:A:251:SER:HB2	1:A:256:LEU:HG	1.85	0.57
1:B:147:ASN:HB2	1:B:152:LEU:CD1	2.34	0.57
1:B:73:THR:HG23	2:B:563:HOH:O	2.03	0.56
1:D:112:LEU:HD23	1:D:113:PRO:HD2	1.86	0.56
1:C:19:ILE:HD12	1:C:71:SER:HA	1.87	0.56
1:A:43:GLU:OE1	2:A:430:HOH:O	2.18	0.56
1:C:363:GLY:O	1:C:364:GLU:C	2.44	0.56
1:B:228:MET:CE	1:B:281:ILE:HG12	2.35	0.56
1:D:275:ASN:HB3	2:D:492:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLN:NE2	1:B:323:ARG:NH1	2.53	0.55
1:D:348:ASN:HD21	1:D:380:ASP:HB2	1.71	0.55
1:D:52:ALA:HB2	1:D:109:PHE:CE1	2.42	0.55
1:C:362:ILE:HD12	1:C:372:LYS:HG2	1.89	0.55
1:D:251:SER:HB2	1:D:256:LEU:HG	1.89	0.54
1:C:12:ALA:O	1:C:13:PRO:C	2.44	0.54
1:D:372:LYS:NZ	2:D:487:HOH:O	2.40	0.54
1:B:332:GLN:HG3	1:B:343:VAL:HB	1.90	0.54
1:D:348:ASN:ND2	1:D:380:ASP:HB2	2.22	0.54
1:C:14:PRO:HG2	1:C:378:SER:C	2.28	0.54
1:B:19:ILE:CD1	1:B:71:SER:HA	2.38	0.54
1:A:51:ASP:HB3	1:C:51:ASP:HB3	1.90	0.54
1:C:354:ARG:CZ	1:C:356:THR:HG21	2.37	0.54
1:C:123:LYS:HE2	1:C:175:LYS:O	2.08	0.54
1:B:41:ARG:NH1	1:B:44:ASP:OD2	2.36	0.53
1:A:137:MET:HE3	1:A:137:MET:CA	2.31	0.53
1:D:86:GLY:O	1:D:87:MET:CG	2.56	0.53
1:C:375:GLU:OE2	1:C:375:GLU:CA	2.54	0.53
1:B:217:ARG:NH2	1:B:219:THR:HG22	2.24	0.53
1:D:16:LYS:HA	1:D:347:ASN:HD21	1.73	0.53
1:D:344:THR:OG1	1:D:348:ASN:HB2	2.09	0.53
1:D:294:ASP:N	1:D:294:ASP:OD2	2.42	0.53
1:B:121:ARG:HB3	1:B:137:MET:HG2	1.91	0.53
1:D:16:LYS:HA	1:D:347:ASN:ND2	2.24	0.53
1:D:243:GLY:HA3	1:D:277:PHE:CD2	2.43	0.53
1:C:251:SER:HB2	1:C:256:LEU:HG	1.91	0.52
1:C:366:VAL:HG23	1:C:368:ARG:HE	1.74	0.52
1:C:27:SER:HB2	1:C:39:TRP:CE2	2.45	0.52
1:A:323:ARG:HG2	2:A:439:HOH:O	2.09	0.52
1:D:129:ASP:HB2	1:D:181:ALA:O	2.10	0.52
1:A:41:ARG:NH2	1:A:43:GLU:OE2	2.38	0.52
1:D:86:GLY:C	1:D:87:MET:CG	2.78	0.52
1:C:17:VAL:HG21	1:C:349:VAL:HG21	1.91	0.52
1:D:198:TRP:CH2	1:D:200:ARG:HB2	2.45	0.51
1:A:177:VAL:HG12	1:A:186:ALA:HB2	1.93	0.51
1:B:34:ASP:O	1:B:35:ILE:HD13	2.11	0.50
1:D:212:ARG:HH11	1:D:212:ARG:HG2	1.77	0.50
1:D:173:ARG:HG3	1:D:173:ARG:HH11	1.77	0.49
1:D:27:SER:HB2	1:D:39:TRP:CE2	2.47	0.49
1:C:12:ALA:O	1:C:13:PRO:O	2.30	0.49
1:D:116:ALA:HB1	2:D:447:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:HB1	1:A:13:PRO:HD2	1.95	0.49
1:C:366:VAL:HG23	1:C:368:ARG:NE	2.28	0.49
1:B:111:PRO:O	1:B:112:LEU:HD23	2.13	0.49
1:B:51:ASP:OD1	1:B:55:ARG:NH2	2.46	0.49
1:C:129:ASP:HB2	1:C:181:ALA:O	2.13	0.49
1:B:232:GLY:HA3	1:B:235:HIS:CE1	2.48	0.48
1:D:18:LEU:HD21	1:D:32:SER:HA	1.94	0.48
1:D:165:LYS:CD	1:D:167:GLN:NE2	2.76	0.48
1:A:239:VAL:HG23	1:A:281:ILE:HD13	1.94	0.48
1:A:75:GLY:HA3	1:A:78:HIS:CE1	2.49	0.48
1:C:348:ASN:ND2	1:C:380:ASP:OD2	2.47	0.48
1:A:225:LYS:HD2	1:A:241:TYR:CE2	2.48	0.48
1:B:248:TYR:CB	2:B:532:HOH:O	2.44	0.47
1:D:232:GLY:HA3	1:D:235:HIS:CE1	2.49	0.47
1:D:16:LYS:O	1:D:32:SER:N	2.40	0.47
1:A:291:LEU:HD12	1:A:296:LYS:O	2.14	0.47
1:C:269:LYS:NZ	2:C:493:HOH:O	2.46	0.47
1:C:105:SER:H	1:D:252:LYS:NZ	2.12	0.47
1:C:228:MET:HG2	1:C:239:VAL:HB	1.96	0.47
1:D:285:PHE:HB2	1:D:337:TRP:HA	1.95	0.47
1:B:17:VAL:HG21	1:B:349:VAL:HG21	1.96	0.47
1:D:133:LEU:HD21	1:D:184:THR:HG21	1.96	0.47
1:B:318:SER:OG	1:C:12:ALA:HB3	2.14	0.47
1:A:12:ALA:N	2:A:482:HOH:O	2.47	0.47
1:A:220:SER:O	1:A:221:THR:CG2	2.63	0.47
1:C:133:LEU:HD21	1:C:184:THR:HG21	1.97	0.46
1:B:52:ALA:HB2	1:B:109:PHE:CE1	2.51	0.46
1:C:349:VAL:HG12	1:C:374:ILE:HD12	1.97	0.46
1:B:228:MET:HE2	1:B:281:ILE:HG12	1.96	0.46
1:B:21:SER:HB3	1:B:74:CYS:SG	2.56	0.46
1:D:52:ALA:HB2	1:D:109:PHE:HE1	1.80	0.45
1:A:221:THR:CG2	1:A:221:THR:O	2.55	0.45
1:B:15:ARG:HD3	1:B:32:SER:O	2.16	0.45
1:B:224:GLU:HG3	1:B:246:TYR:OH	2.15	0.45
1:C:121:ARG:HG2	1:C:137:MET:HG3	1.98	0.45
1:B:372:LYS:HD3	2:B:438:HOH:O	2.15	0.45
1:B:204:LEU:HD12	2:B:501:HOH:O	2.15	0.45
1:B:321:GLN:NE2	1:B:323:ARG:HH11	2.13	0.45
1:C:296:LYS:CG	1:C:321:GLN:OE1	2.64	0.45
1:C:118:HIS:CE1	2:C:537:HOH:O	2.69	0.45
1:D:305:PHE:CD1	1:D:354:ARG:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:VAL:CG2	1:C:368:ARG:HE	2.30	0.45
1:B:184:THR:HG21	1:B:196:TRP:CZ2	2.51	0.45
1:A:17:VAL:HG21	1:A:349:VAL:HG21	1.99	0.45
1:A:354:ARG:CZ	1:A:356:THR:HG21	2.46	0.45
1:A:285:PHE:HB2	1:A:337:TRP:CA	2.39	0.44
1:B:19:ILE:HB	1:B:30:LEU:HB3	1.99	0.44
1:C:310:VAL:HG11	1:C:320:VAL:CG1	2.47	0.44
1:D:20:ILE:HD12	1:D:20:ILE:C	2.35	0.44
1:B:108:LEU:HD13	1:B:112:LEU:HB2	2.00	0.44
1:D:376:ALA:C	1:D:377:LEU:HD23	2.37	0.44
1:C:225:LYS:HD3	1:C:241:TYR:CE2	2.52	0.44
1:A:220:SER:O	1:A:221:THR:HG22	2.17	0.44
1:B:273:LEU:HD13	1:B:278:ILE:HD11	1.99	0.44
1:C:71:SER:HB3	1:C:82:TYR:CE2	2.52	0.44
1:C:228:MET:HE2	1:C:228:MET:HB2	1.93	0.43
1:A:137:MET:CA	1:A:137:MET:CE	2.95	0.43
1:D:61:LEU:CD2	1:D:63:ALA:HB3	2.48	0.43
1:A:251:SER:CB	1:A:256:LEU:HG	2.48	0.43
1:D:237:ILE:CG2	1:D:245:LEU:HD11	2.49	0.43
1:D:60:GLN:NE2	1:D:65:ASP:OD2	2.52	0.43
1:D:256:LEU:HD12	1:D:264:HIS:HD2	1.83	0.43
1:B:147:ASN:HB2	1:B:152:LEU:HD12	1.99	0.43
1:D:127:CYS:HG	1:D:132:CYS:HG	1.63	0.43
1:C:332:GLN:O	1:C:342:ALA:HA	2.19	0.43
1:C:125:ILE:HD13	1:C:134:ALA:HB2	2.01	0.42
1:B:70:VAL:HG13	2:B:526:HOH:O	2.18	0.42
1:B:251:SER:HB2	1:B:256:LEU:HG	2.01	0.42
1:A:349:VAL:HG12	1:A:374:ILE:HD12	2.01	0.42
1:D:372:LYS:HB2	2:D:496:HOH:O	2.19	0.42
1:A:70:VAL:HG21	1:A:84:GLN:CG	2.45	0.42
1:B:27:SER:HB2	1:B:39:TRP:CE2	2.53	0.42
1:D:71:SER:OG	1:D:82:TYR:CE2	2.68	0.42
1:D:15:ARG:HG2	1:D:32:SER:O	2.19	0.42
1:A:110:THR:HG21	1:C:110:THR:HG21	2.00	0.42
1:B:176:MET:HB3	1:B:187:VAL:HG22	2.01	0.42
1:C:180:GLY:HA3	1:C:183:HIS:CE1	2.55	0.42
1:D:20:ILE:CD1	1:D:20:ILE:O	2.58	0.42
1:B:34:ASP:OD2	1:B:68:GLN:HA	2.20	0.42
1:C:18:LEU:N	1:C:18:LEU:HD13	2.34	0.42
1:A:212:ARG:HE	1:A:216:GLU:CD	2.23	0.42
1:C:202:GLY:HA3	1:C:265:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LYS:CE	1:D:167:GLN:NE2	2.83	0.42
1:B:336:GLY:HA3	1:B:339:HIS:CE1	2.55	0.41
1:D:181:ALA:HB2	1:D:233:TRP:CD1	2.55	0.41
1:C:16:LYS:H	1:C:16:LYS:HG3	1.64	0.41
1:B:326:ASP:HB2	1:B:346:ARG:HH21	1.84	0.41
1:B:363:GLY:O	1:B:364:GLU:C	2.58	0.41
1:D:338:ARG:NH2	2:D:416:HOH:O	2.52	0.41
1:A:137:MET:HA	1:A:137:MET:CE	2.40	0.41
1:D:286:ARG:HD2	1:D:302:TRP:CE3	2.55	0.41
1:D:112:LEU:CD2	1:D:113:PRO:HD2	2.50	0.41
1:A:95:GLY:HA2	1:A:100:LEU:HG	2.02	0.41
1:A:346:ARG:O	1:A:347:ASN:HB2	2.21	0.41
1:C:354:ARG:NH2	1:C:356:THR:HG21	2.35	0.41
1:C:121:ARG:NH2	1:C:138:GLU:OE2	2.53	0.41
1:A:224:GLU:OE2	2:A:470:HOH:O	2.21	0.41
1:B:98:GLY:HA3	1:B:161:LEU:HD23	2.03	0.41
1:C:290:ALA:O	1:C:297:LEU:HD12	2.20	0.41
1:B:243:GLY:HA3	1:B:277:PHE:CD2	2.56	0.41
1:A:321:GLN:NE2	2:A:512:HOH:O	2.48	0.41
1:D:296:LYS:HG2	2:D:533:HOH:O	2.21	0.41
1:A:31:LEU:HD21	1:A:377:LEU:HD22	2.03	0.40
1:B:24:ALA:HA	1:B:337:TRP:CG	2.56	0.40
1:C:183:HIS:CG	1:C:203:ASN:HD22	2.39	0.40
1:A:173:ARG:HE	1:A:173:ARG:HB3	1.75	0.40
1:A:147:ASN:O	1:A:157:THR:HA	2.20	0.40
1:D:243:GLY:HA3	1:D:277:PHE:CE2	2.57	0.40
1:A:225:LYS:HE3	2:A:458:HOH:O	2.21	0.40
1:C:303:ASN:ND2	1:C:312:ASN:O	2.54	0.40
1:C:41:ARG:NH1	1:C:46:GLN:HE22	2.19	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:LYS:NZ	1:D:84:GLN:OE1[1_465]	2.04	0.16
1:A:167:GLN:OE1	1:B:55:ARG:NH1[1_455]	2.12	0.08

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	368/370 (100%)	360 (98%)	8 (2%)	0	100	100
1	B	366/370 (99%)	358 (98%)	8 (2%)	0	100	100
1	C	369/370 (100%)	359 (97%)	8 (2%)	2 (0%)	34	26
1	D	366/370 (99%)	351 (96%)	15 (4%)	0	100	100
All	All	1469/1480 (99%)	1428 (97%)	39 (3%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	13	PRO
1	C	364	GLU

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	292/292 (100%)	279 (96%)	13 (4%)	34	29
1	B	290/292 (99%)	277 (96%)	13 (4%)	34	29
1	C	293/292 (100%)	273 (93%)	20 (7%)	20	13
1	D	291/292 (100%)	270 (93%)	21 (7%)	18	12
All	All	1166/1168 (100%)	1099 (94%)	67 (6%)	25	19

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	25	SER
1	A	46	GLN
1	A	85	SER
1	A	133	LEU
1	A	158	GLU
1	A	173	ARG
1	A	190	ASP
1	A	221	THR
1	A	233	TRP
1	A	323	ARG
1	A	332	GLN
1	A	372	LYS
1	B	15	ARG
1	B	21	SER
1	B	32	SER
1	B	73	THR
1	B	85	SER
1	B	120	ILE
1	B	130	SER
1	B	182	GLU
1	B	228	MET
1	B	233	TRP
1	B	276	SER
1	B	332	GLN
1	B	346	ARG
1	C	18	LEU
1	C	84	GLN
1	C	88	GLU
1	C	121	ARG
1	C	129	ASP
1	C	158	GLU
1	C	167	GLN
1	C	173	ARG
1	C	176	MET
1	C	216	GLU
1	C	219	THR
1	C	224	GLU
1	C	233	TRP
1	C	271	GLU
1	C	314	LEU
1	C	346	ARG
1	C	365	SER

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Mol	Chain	Res	Type
1	C	368	ARG
1	C	372	LYS
1	C	373	ILE
1	D	18	LEU
1	D	34	ASP
1	D	53	GLU
1	D	71	SER
1	D	87	MET
1	D	106	SER
1	D	110	THR
1	D	125	ILE
1	D	129	ASP
1	D	133	LEU
1	D	170	GLU
1	D	173	ARG
1	D	216	GLU
1	D	233	TRP
1	D	270	LEU
1	D	279	SER
1	D	294	ASP
1	D	346	ARG
1	D	364	GLU
1	D	372	LYS
1	D	380	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	321	GLN
1	B	164	GLN
1	B	321	GLN
1	C	347	ASN
1	D	167	GLN
1	D	264	HIS
1	D	321	GLN
1	D	332	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	370/370 (100%)	0.06	8 (2%)	65	66	15, 25, 48, 113	0
1	B	368/370 (99%)	0.14	8 (2%)	65	66	15, 27, 57, 78	0
1	C	370/370 (100%)	0.19	6 (1%)	74	75	17, 28, 52, 119	0
1	D	368/370 (99%)	0.36	15 (4%)	41	42	20, 33, 60, 112	0
All	All	1476/1480 (99%)	0.19	37 (2%)	61	61	15, 29, 57, 119	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	12	ALA	5.5
1	A	222	GLY	4.1
1	D	381	GLY	3.8
1	C	190	ASP	3.6
1	D	364	GLU	3.6
1	A	221	THR	3.5
1	B	222	GLY	3.4
1	D	53	GLU	3.4
1	D	15	ARG	3.2
1	A	12	ALA	3.1
1	D	366	VAL	3.1
1	C	381	GLY	3.1
1	C	364	GLU	3.0
1	D	275	ASN	2.7
1	A	223	GLY	2.6
1	B	220	SER	2.6
1	C	379	VAL	2.5
1	D	298	TYR	2.4
1	B	34	ASP	2.4
1	D	87	MET	2.4
1	B	364	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	120	ILE	2.3
1	D	377	LEU	2.3
1	D	16	LYS	2.3
1	A	345	GLU	2.3
1	D	375	GLU	2.3
1	C	16	LYS	2.2
1	A	220	SER	2.2
1	A	13	PRO	2.2
1	B	380	ASP	2.2
1	D	337	TRP	2.2
1	D	222	GLY	2.2
1	B	326	ASP	2.1
1	B	223	GLY	2.1
1	A	346	ARG	2.0
1	D	324	PHE	2.0
1	B	14	PRO	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.