Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 01:15 PM EDT

PDB ID	:	3US1
Title	:	Structure of p63 DNA Binding Domain in Complex with a 22 Base Pair Response Element Containing a Two Base Pair "GC" Spacer Between Half Sites
Authors	:	Chen, C.; Herzberg, O.
Deposited on	:	2011-11-22
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
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:

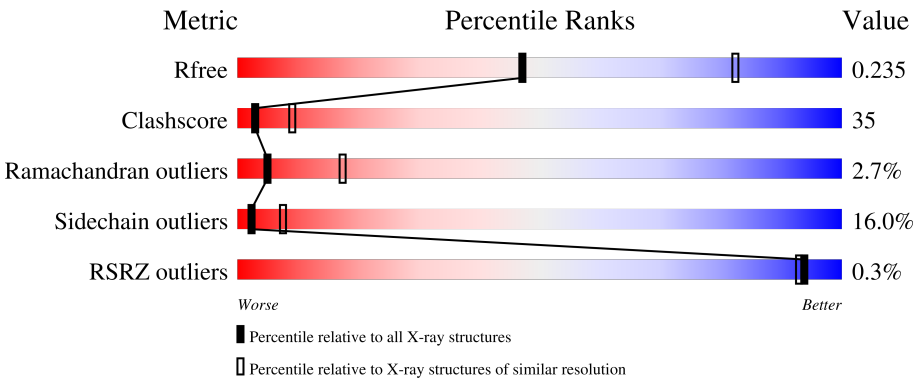
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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	203	42% 43% 10% 5%
1	D	203	39% 39% 11% 10%
2	F	22	64% 32% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3538 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 Tumor protein 63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	193	1497	938	263	284	12	0	0	0
1	D	182	1417	891	250	264	12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	GLY	-	expression tag	UNP Q9H3D4
A	122	SER	-	expression tag	UNP Q9H3D4
A	123	HIS	-	expression tag	UNP Q9H3D4
A	124	MET	-	expression tag	UNP Q9H3D4
A	125	ALA	-	expression tag	UNP Q9H3D4
A	126	SER	-	expression tag	UNP Q9H3D4
D	121	GLY	-	expression tag	UNP Q9H3D4
D	122	SER	-	expression tag	UNP Q9H3D4
D	123	HIS	-	expression tag	UNP Q9H3D4
D	124	MET	-	expression tag	UNP Q9H3D4
D	125	ALA	-	expression tag	UNP Q9H3D4
D	126	SER	-	expression tag	UNP Q9H3D4

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*TP*GP*CP*AP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	22	448	217	80	130	21	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
			Total	Zn		
3	D	1	1	1	0	0

- Molecule 4 is water.

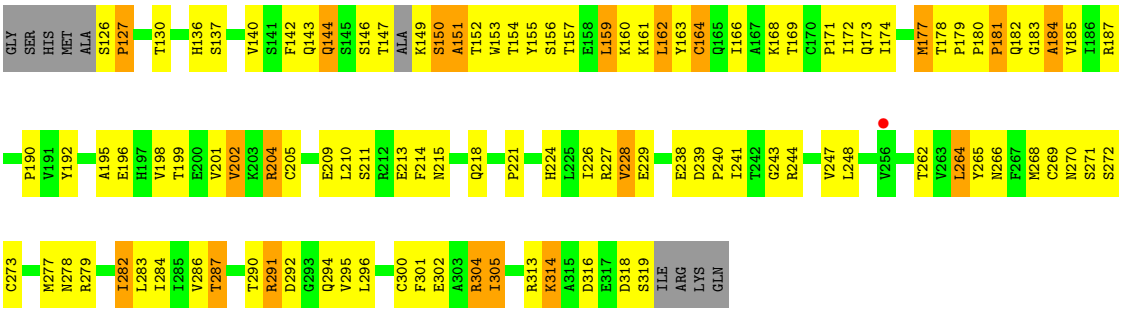
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	78	78	78	0	0
			Total	O		
4	D	80	80	80	0	0
			Total	O		
4	F	16	16	16	0	0

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.

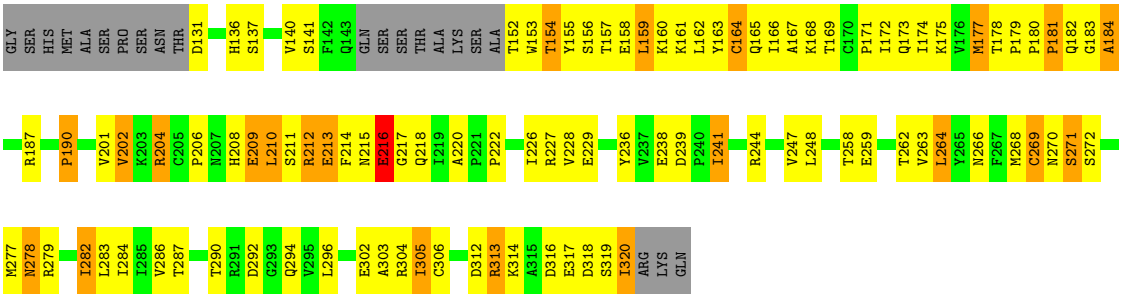
• Molecule 1: Tumor protein 63

Chain A: 42% 43% 10% 5%



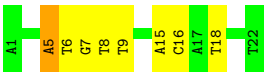
• Molecule 1: Tumor protein 63

Chain D: 39% 39% 11% 10%



• Molecule 2: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*TP*GP*CP*AP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'

Chain F: 64% 32% 5%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	84.95Å 101.22Å 71.50Å 90.00° 122.78° 90.00°	Depositor
Resolution (Å)	19.61 – 2.80 19.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.61-2.80) 98.3 (19.61-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.202 , 0.234 0.203 , 0.235	Depositor DCC
R_{free} test set	1106 reflections (8.96%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3538	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.64	1/1532 (0.1%)	0.83	0/2083
1	D	0.55	0/1451	0.76	0/1974
2	F	0.46	0/502	0.76	0/773
All	All	0.58	1/3485 (0.0%)	0.79	0/4830

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	CYS	CB-SG	-6.03	1.72	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	5	DA	Sidechain

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	1497	0	1456	120	0
1	D	1417	0	1377	94	0
2	F	448	0	252	12	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	78	0	0	10	0
4	D	80	0	0	2	0
4	F	16	0	0	1	0
All	All	3538	0	3085	224	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 35.

All (224) 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:D:131:ASP:N	4:D:61:HOH:O	1.65	1.24
1:D:137:SER:CB	1:D:177:MET:HG3	1.75	1.15
1:A:126:SER:N	4:A:45:HOH:O	1.86	1.07
1:A:172:ILE:HD12	1:A:265:TYR:HD2	1.21	1.06
1:A:290:THR:HG22	1:A:294:GLN:H	1.20	1.06
1:D:290:THR:HG22	1:D:294:GLN:H	1.13	1.05
1:D:137:SER:HB2	1:D:177:MET:CG	1.89	1.02
1:A:240:PRO:HG2	1:A:241:ILE:HD12	1.44	0.99
1:D:204:ARG:HD2	1:D:268:MET:HB2	1.47	0.96
1:D:137:SER:HB2	1:D:177:MET:HG3	0.96	0.94
1:D:290:THR:HG22	1:D:294:GLN:N	1.84	0.92
1:D:239:ASP:OD1	1:D:241:ILE:HG13	1.70	0.91
1:A:295:VAL:HG12	4:A:34:HOH:O	1.71	0.90
1:A:172:ILE:HD12	1:A:265:TYR:CD2	2.11	0.86
1:A:143:GLN:HA	1:A:144:GLN:NE2	1.93	0.83
1:A:144:GLN:CD	1:A:144:GLN:H	1.75	0.82
1:A:168:LYS:O	4:A:54:HOH:O	1.97	0.82
1:A:137:SER:HB2	1:A:177:MET:HB2	1.59	0.82
1:A:204:ARG:HD2	1:A:268:MET:HB2	1.59	0.81
1:D:290:THR:CG2	1:D:294:GLN:H	1.92	0.81
1:A:169:THR:HB	1:A:229:GLU:OE2	1.80	0.80
1:A:290:THR:HG22	1:A:294:GLN:N	1.96	0.79
1:D:175:LYS:HD3	1:D:259:GLU:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLN:NE2	1:A:144:GLN:H	1.81	0.78
1:D:271:SER:O	1:D:279:ARG:HA	1.83	0.77
1:A:204:ARG:NH2	1:A:215:ASN:HD21	1.82	0.76
1:D:277:MET:SD	1:D:282:ILE:HG21	2.26	0.75
1:D:212:ARG:HH11	1:D:216:GLU:HG2	1.50	0.75
2:F:5:DA:H2"	2:F:6:DT:C5'	2.16	0.74
1:D:216:GLU:OE1	1:D:216:GLU:HA	1.87	0.74
1:A:290:THR:CG2	1:A:294:GLN:H	2.00	0.74
1:D:136:HIS:CE1	1:D:180:PRO:HA	2.24	0.73
1:D:272:SER:HA	1:D:279:ARG:H	1.56	0.71
1:A:196:GLU:HA	1:D:216:GLU:HG3	1.71	0.71
1:A:277:MET:SD	1:A:282:ILE:HG21	2.30	0.71
1:A:163:TYR:CE2	1:A:313:ARG:HA	2.24	0.71
1:A:195:ALA:HB3	1:D:217:GLY:HA3	1.71	0.70
1:D:226:ILE:HD11	1:D:284:ILE:HD12	1.72	0.70
1:A:272:SER:HA	1:A:279:ARG:H	1.58	0.69
1:D:269:CYS:O	1:D:305:ILE:HD11	1.91	0.69
1:D:169:THR:HB	1:D:229:GLU:OE2	1.93	0.68
2:F:5:DA:H2"	2:F:6:DT:H5'	1.74	0.68
1:D:220:ALA:HB2	1:D:236:TYR:CZ	2.29	0.68
1:D:220:ALA:HB2	1:D:236:TYR:CE1	2.29	0.68
1:D:269:CYS:O	1:D:305:ILE:CD1	2.42	0.68
1:A:305:ILE:O	4:A:56:HOH:O	2.12	0.67
1:A:161:LYS:HG3	1:A:302:GLU:HB3	1.78	0.65
1:A:290:THR:HG23	1:A:292:ASP:H	1.62	0.65
1:D:164:CYS:O	1:D:305:ILE:HA	1.97	0.64
1:D:258:THR:HG22	1:D:259:GLU:H	1.61	0.64
1:A:204:ARG:HD2	1:A:268:MET:CB	2.27	0.64
2:F:5:DA:H2"	2:F:6:DT:H5"	1.80	0.63
1:D:163:TYR:CE2	1:D:313:ARG:HA	2.34	0.63
1:D:183:GLY:O	1:D:184:ALA:O	2.15	0.63
1:A:218:GLN:NE2	1:A:218:GLN:HA	2.13	0.63
1:A:177:MET:HA	1:A:177:MET:CE	2.30	0.62
1:D:313:ARG:O	1:D:317:GLU:HG3	1.99	0.62
1:D:141:SER:O	1:D:173:GLN:HB2	1.99	0.62
1:A:154:THR:HG23	1:A:163:TYR:HB2	1.80	0.61
1:A:156:SER:OG	1:A:159:LEU:HB2	2.01	0.61
1:A:271:SER:O	1:A:279:ARG:HA	2.02	0.60
1:A:182:GLN:HA	1:A:182:GLN:NE2	2.17	0.60
1:D:156:SER:HA	1:D:313:ARG:NH2	2.16	0.60
1:A:270:ASN:HA	1:A:305:ILE:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:THR:CG2	1:A:294:GLN:HB3	2.31	0.60
2:F:18:DT:OP1	4:F:33:HOH:O	2.17	0.60
1:D:290:THR:CG2	1:D:294:GLN:HB3	2.32	0.60
1:A:155:TYR:CE2	1:A:157:THR:HA	2.37	0.59
1:D:180:PRO:O	1:D:181:PRO:O	2.20	0.59
1:D:140:VAL:HG12	1:D:174:ILE:HD13	1.82	0.59
1:A:282:ILE:HG13	1:A:283:LEU:N	2.17	0.59
1:D:312:ASP:O	1:D:316:ASP:HB2	2.03	0.59
1:A:149:LYS:HA	4:A:342:HOH:O	2.03	0.58
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.68	0.57
1:D:187:ARG:CZ	1:D:248:LEU:HD21	2.33	0.57
1:D:278:ASN:O	1:D:279:ARG:HG2	2.04	0.57
1:A:166:ILE:HA	1:A:305:ILE:CD1	2.34	0.57
1:A:244:ARG:HH11	1:A:244:ARG:HG2	1.69	0.57
1:A:187:ARG:CZ	1:A:248:LEU:HD21	2.33	0.57
1:A:154:THR:CG2	1:A:163:TYR:HB2	2.34	0.57
2:F:7:DG:H2"	2:F:8:DT:H5'	1.85	0.57
1:A:221:PRO:HB2	1:A:224:HIS:CD2	2.40	0.57
1:D:204:ARG:HD2	1:D:268:MET:CB	2.30	0.56
1:D:283:LEU:HB3	1:D:302:GLU:HA	1.87	0.56
2:F:7:DG:H1'	2:F:8:DT:H5"	1.87	0.56
1:A:166:ILE:HG13	1:A:305:ILE:HD11	1.86	0.56
1:D:290:THR:HG21	1:D:294:GLN:HB3	1.87	0.56
1:D:155:TYR:CE2	1:D:157:THR:HA	2.41	0.56
1:D:211:SER:O	1:D:212:ARG:C	2.43	0.56
1:A:283:LEU:HB3	1:A:302:GLU:HA	1.88	0.55
1:A:146:SER:O	1:A:147:THR:HG23	2.06	0.55
1:D:187:ARG:HB3	1:D:287:THR:HG23	1.88	0.55
1:D:258:THR:HG22	1:D:259:GLU:N	2.21	0.55
1:A:142:PHE:CE1	1:A:172:ILE:HG12	2.41	0.55
1:A:149:LYS:N	4:A:335:HOH:O	2.40	0.55
1:A:201:VAL:HG12	1:A:202:VAL:N	2.22	0.55
1:D:187:ARG:HB2	1:D:248:LEU:HD22	1.89	0.55
1:A:143:GLN:N	1:A:173:GLN:OE1	2.39	0.55
1:A:226:ILE:HD11	1:A:284:ILE:HD12	1.89	0.55
1:A:180:PRO:O	1:A:181:PRO:O	2.25	0.54
1:A:290:THR:HG21	1:A:294:GLN:HB3	1.89	0.54
1:D:182:GLN:HE21	1:D:182:GLN:HA	1.72	0.54
1:D:213:GLU:O	1:D:214:PHE:HB2	2.08	0.54
1:A:210:LEU:O	1:A:211:SER:C	2.46	0.54
1:A:228:VAL:HG12	1:A:247:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:LYS:HD3	1:D:163:TYR:CZ	2.44	0.53
1:A:155:TYR:HE2	1:A:157:THR:HA	1.74	0.53
2:F:8:DT:C6	2:F:9:DT:H72	2.44	0.52
1:D:171:PRO:HA	1:D:264:LEU:HD12	1.92	0.52
1:A:187:ARG:HB3	1:A:287:THR:HG23	1.91	0.51
1:D:201:VAL:HG12	1:D:202:VAL:N	2.25	0.51
1:A:209:GLU:HG2	1:A:209:GLU:O	2.09	0.51
1:A:187:ARG:HB2	1:A:248:LEU:CD2	2.40	0.50
1:A:244:ARG:HG2	1:A:244:ARG:NH1	2.25	0.50
1:A:291:ARG:NH1	1:A:291:ARG:HG3	2.26	0.50
1:A:150:SER:O	1:A:152:THR:N	2.43	0.50
1:A:162:LEU:HD12	1:A:301:PHE:HE2	1.75	0.50
1:A:144:GLN:CD	1:A:144:GLN:N	2.57	0.50
1:A:241:ILE:HD12	1:A:241:ILE:H	1.77	0.50
1:D:290:THR:HG23	1:D:292:ASP:H	1.76	0.50
1:D:172:ILE:HG22	1:D:263:VAL:HB	1.94	0.50
1:D:204:ARG:NH1	1:D:208:HIS:HB3	2.27	0.50
1:D:152:THR:HG23	1:D:153:TRP:HD1	1.77	0.50
2:F:5:DA:C2'	2:F:6:DT:H5"	2.40	0.50
1:A:136:HIS:CE1	1:A:180:PRO:HA	2.47	0.50
1:D:214:PHE:O	1:D:218:GLN:HG3	2.12	0.50
1:A:164:CYS:O	1:A:305:ILE:HA	2.11	0.49
1:A:190:PRO:C	1:A:202:VAL:HG21	2.32	0.49
1:D:187:ARG:NH1	1:D:248:LEU:HD21	2.27	0.49
1:A:143:GLN:HB3	1:A:173:GLN:NE2	2.28	0.49
1:A:143:GLN:HB3	1:A:173:GLN:OE1	2.13	0.49
1:A:187:ARG:NH1	1:A:248:LEU:HD21	2.28	0.49
1:D:169:THR:HA	1:D:266:ASN:ND2	2.28	0.49
1:D:156:SER:OG	1:D:159:LEU:HB2	2.13	0.48
1:A:183:GLY:O	1:A:184:ALA:C	2.52	0.48
1:A:241:ILE:HD12	1:A:241:ILE:N	2.27	0.48
1:A:140:VAL:HG12	1:A:174:ILE:HD13	1.94	0.48
1:A:227:ARG:NH1	1:A:268:MET:HE1	2.29	0.48
1:D:169:THR:HG22	4:D:14:HOH:O	2.12	0.48
1:D:215:ASN:O	1:D:216:GLU:C	2.50	0.48
2:F:15:DA:H1'	2:F:16:DC:H5'	1.95	0.48
1:A:240:PRO:HG2	1:A:241:ILE:CD1	2.30	0.48
1:D:183:GLY:O	1:D:184:ALA:C	2.52	0.48
1:A:190:PRO:O	1:A:202:VAL:HG21	2.14	0.48
1:A:314:LYS:HE3	1:A:318:ASP:OD2	2.13	0.48
1:A:166:ILE:HA	1:A:305:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:ASP:C	1:D:320:ILE:H	2.17	0.47
1:A:149:LYS:C	1:A:151:ALA:N	2.68	0.47
1:A:162:LEU:HD12	1:A:301:PHE:CE2	2.49	0.47
1:D:175:LYS:CD	1:D:259:GLU:O	2.59	0.47
1:D:270:ASN:C	1:D:272:SER:H	2.17	0.47
1:A:201:VAL:CG1	1:A:202:VAL:N	2.77	0.47
1:A:171:PRO:HA	1:A:264:LEU:HD12	1.96	0.47
1:A:209:GLU:C	1:A:210:LEU:HD12	2.35	0.47
1:D:153:TRP:HB3	1:D:164:CYS:HB2	1.96	0.47
1:D:140:VAL:HG12	1:D:174:ILE:CD1	2.45	0.47
1:A:192:TYR:OH	4:A:55:HOH:O	2.18	0.46
1:D:161:LYS:HE3	1:D:302:GLU:OE2	2.16	0.46
1:A:127:PRO:HA	4:A:72:HOH:O	2.16	0.46
1:A:153:TRP:HB3	1:A:164:CYS:HB2	1.97	0.46
1:D:272:SER:HA	1:D:279:ARG:N	2.26	0.46
1:D:155:TYR:OH	1:D:160:LYS:HA	2.15	0.46
1:A:169:THR:HA	1:A:266:ASN:ND2	2.31	0.46
1:D:216:GLU:OE1	1:D:216:GLU:CA	2.60	0.46
1:D:228:VAL:HG12	1:D:247:VAL:HG21	1.98	0.46
1:A:143:GLN:HB3	1:A:173:GLN:HE22	1.79	0.46
1:A:209:GLU:O	1:A:209:GLU:CG	2.64	0.45
1:D:201:VAL:CG1	1:D:202:VAL:N	2.79	0.45
1:A:213:GLU:O	1:A:214:PHE:HB2	2.17	0.45
1:A:291:ARG:HG3	1:A:291:ARG:HH11	1.81	0.45
1:D:244:ARG:HG2	1:D:244:ARG:HH11	1.82	0.45
1:D:182:GLN:HA	1:D:182:GLN:NE2	2.32	0.45
1:D:206:PRO:O	1:D:210:LEU:HD12	2.17	0.45
1:A:143:GLN:CB	1:A:173:GLN:HE22	2.30	0.44
1:A:140:VAL:HG12	1:A:174:ILE:CD1	2.47	0.44
1:A:166:ILE:HA	1:A:305:ILE:HD11	1.99	0.44
1:D:190:PRO:HG2	1:D:202:VAL:CG2	2.47	0.44
1:A:187:ARG:HB2	1:A:248:LEU:HD22	2.00	0.44
2:F:7:DG:H2"	2:F:8:DT:C5'	2.47	0.44
2:F:8:DT:H2'	2:F:9:DT:H72	1.99	0.44
1:A:149:LYS:CB	4:A:335:HOH:O	2.65	0.43
1:A:161:LYS:HB3	1:A:163:TYR:HE1	1.84	0.43
1:D:190:PRO:C	1:D:202:VAL:HG21	2.39	0.43
1:A:272:SER:HA	1:A:279:ARG:N	2.29	0.43
1:D:209:GLU:O	1:D:222:PRO:HB2	2.18	0.43
1:D:244:ARG:HG2	1:D:244:ARG:NH1	2.33	0.43
1:A:156:SER:O	1:A:160:LYS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:SER:HB2	1:A:177:MET:CB	2.42	0.43
1:D:154:THR:HG23	1:D:163:TYR:HB2	2.01	0.43
1:D:284:ILE:HG12	1:D:303:ALA:HB2	2.01	0.43
1:A:163:TYR:N	1:A:163:TYR:CD1	2.87	0.42
1:A:295:VAL:CG1	4:A:34:HOH:O	2.47	0.42
1:D:282:ILE:HG13	1:D:283:LEU:N	2.34	0.42
1:D:277:MET:O	1:D:278:ASN:C	2.57	0.42
1:A:153:TRP:CE3	1:A:154:THR:N	2.87	0.42
1:A:239:ASP:O	1:A:243:GLY:N	2.47	0.42
1:A:205:CYS:SG	1:A:273:CYS:HB3	2.59	0.42
1:A:277:MET:O	1:A:278:ASN:C	2.58	0.42
1:D:165:GLN:HA	1:D:306:CYS:O	2.20	0.42
1:A:198:VAL:HG23	1:A:199:THR:N	2.35	0.42
1:A:150:SER:O	1:A:150:SER:OG	2.38	0.41
1:A:204:ARG:HH21	1:A:215:ASN:HD21	1.63	0.41
1:D:179:PRO:HA	1:D:180:PRO:HD2	1.94	0.41
1:A:183:GLY:O	1:A:185:VAL:HG13	2.20	0.41
1:D:212:ARG:HD2	1:D:216:GLU:OE2	2.20	0.41
1:A:290:THR:HB	1:A:296:LEU:HD21	2.03	0.41
1:A:179:PRO:HA	1:A:180:PRO:HD2	1.95	0.41
1:D:161:LYS:HG3	1:D:302:GLU:HB3	2.01	0.41
1:A:154:THR:OG1	1:A:313:ARG:NH1	2.53	0.41
1:A:304:ARG:HG3	1:A:304:ARG:NH1	2.34	0.41
1:D:187:ARG:HB2	1:D:248:LEU:CD2	2.50	0.41
1:A:239:ASP:O	1:A:243:GLY:HA2	2.20	0.41
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.77	0.41
1:D:180:PRO:C	1:D:181:PRO:O	2.59	0.41
1:D:227:ARG:HA	1:D:236:TYR:HE2	1.85	0.41
2:F:7:DG:H2"	2:F:8:DT:OP2	2.21	0.41
1:A:162:LEU:CD2	1:A:164:CYS:HB3	2.51	0.40
1:A:177:MET:HA	1:A:177:MET:HE2	2.01	0.40
1:D:166:ILE:O	1:D:168:LYS:N	2.54	0.40
1:D:211:SER:O	1:D:213:GLU:N	2.54	0.40
1:D:264:LEU:HD12	1:D:264:LEU:HA	1.82	0.40
1:A:161:LYS:HB3	1:A:163:TYR:CE1	2.57	0.40
1:A:182:GLN:NE2	1:A:182:GLN:CA	2.80	0.40
1:D:290:THR:HB	1:D:296:LEU:HD21	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	189/203 (93%)	167 (88%)	18 (10%)	4 (2%)	7 23
1	D	178/203 (88%)	152 (85%)	20 (11%)	6 (3%)	3 13
All	All	367/406 (90%)	319 (87%)	38 (10%)	10 (3%)	5 17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ALA
1	A	181	PRO
1	D	181	PRO
1	D	184	ALA
1	D	216	GLU
1	A	127	PRO
1	A	184	ALA
1	D	167	ALA
1	D	319	SER
1	D	212	ARG

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	167/179 (93%)	143 (86%)	24 (14%)	3 10
1	D	157/179 (88%)	129 (82%)	28 (18%)	2 5
All	All	324/358 (90%)	272 (84%)	52 (16%)	2 7

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	THR
1	A	144	GLN
1	A	150	SER
1	A	159	LEU
1	A	162	LEU
1	A	164	CYS
1	A	177	MET
1	A	178	THR
1	A	202	VAL
1	A	204	ARG
1	A	228	VAL
1	A	238	GLU
1	A	262	THR
1	A	264	LEU
1	A	269	CYS
1	A	282	ILE
1	A	286	VAL
1	A	287	THR
1	A	291	ARG
1	A	304	ARG
1	A	305	ILE
1	A	314	LYS
1	A	316	ASP
1	A	319	SER
1	D	154	THR
1	D	158	GLU
1	D	159	LEU
1	D	162	LEU
1	D	164	CYS
1	D	177	MET
1	D	178	THR
1	D	190	PRO
1	D	202	VAL
1	D	204	ARG
1	D	209	GLU
1	D	210	LEU
1	D	213	GLU
1	D	216	GLU
1	D	238	GLU
1	D	241	ILE
1	D	262	THR
1	D	264	LEU

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Mol	Chain	Res	Type
1	D	269	CYS
1	D	271	SER
1	D	278	ASN
1	D	282	ILE
1	D	286	VAL
1	D	304	ARG
1	D	305	ILE
1	D	313	ARG
1	D	314	LYS
1	D	320	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	144	GLN
1	A	182	GLN
1	A	197	HIS
1	A	215	ASN
1	A	245	GLN
1	A	266	ASN
1	D	173	GLN
1	D	182	GLN
1	D	266	ASN

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	193/203 (95%)	-0.51	1 (0%)	91	88	14, 35, 69, 103	0
1	D	182/203 (89%)	-0.31	0	100	100	27, 50, 88, 118	0
2	F	22/22 (100%)	-0.85	0	100	100	26, 42, 49, 55	0
All	All	397/428 (92%)	-0.43	1 (0%)	94	93	14, 43, 78, 118	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	VAL	2.3

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	A	901	1/1	0.96	0.11	35,35,35,35	0
3	ZN	D	901	1/1	0.99	0.11	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.