Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:31 AM GMT

PDB ID	:	2XDN
Title	:	TRANSCRIPTION FACTOR TTGR H67A MUTANT
Authors	:	Daniels, C.; Lu, D.; Zhang, X.; Ramos, J.L.
Deposited on	:	2010-05-04
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:

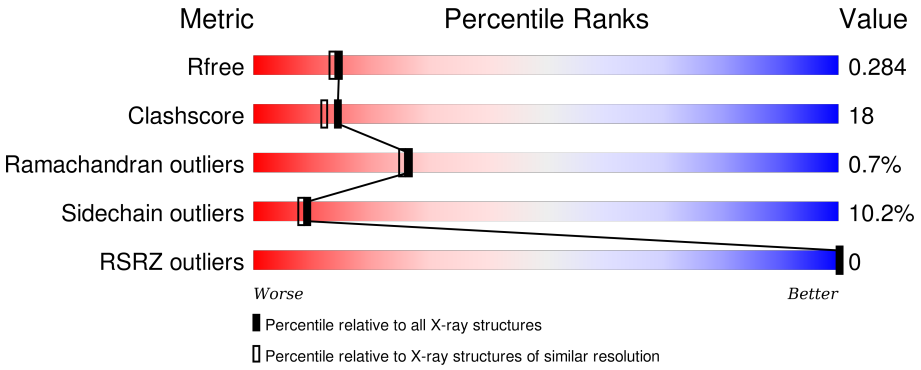
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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))
R_{free}	91344	3774 (2.20-2.20)
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	210	66% 26% 5% •
1	B	210	50% 41% 6% •
1	C	210	63% 30% 5% •
1	D	210	63% 31% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6363 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 HTH-TYPE TRANSCRIPTIONAL REGULATOR TTGR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1577	988	284	297	8			
1	B	205	Total	C	N	O	S	0	0	0
			1580	988	291	293	8			
1	C	206	Total	C	N	O	S	0	0	0
			1605	1002	295	300	8			
1	D	205	Total	C	N	O	S	0	1	0
			1590	994	291	298	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ALA	HIS	ENGINEERED MUTATION	UNP Q9AIU0
B	67	ALA	HIS	ENGINEERED MUTATION	UNP Q9AIU0
C	67	ALA	HIS	ENGINEERED MUTATION	UNP Q9AIU0
D	67	ALA	HIS	ENGINEERED MUTATION	UNP Q9AIU0

- Molecule 2 is water.

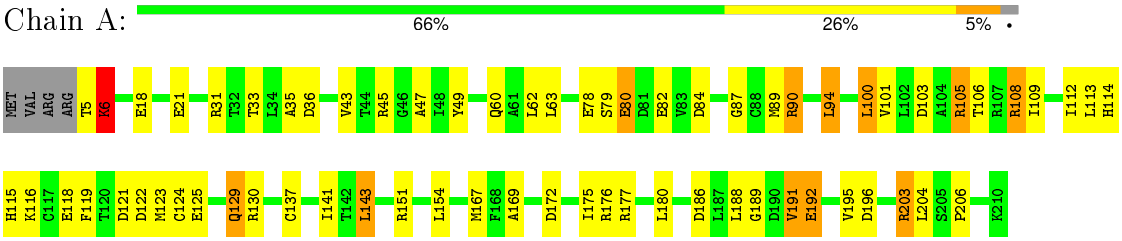
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	4	Total	O	0	0
			4	4		
2	C	3	Total	O	0	0
			3	3		
2	D	2	Total	O	0	0
			2	2		

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.

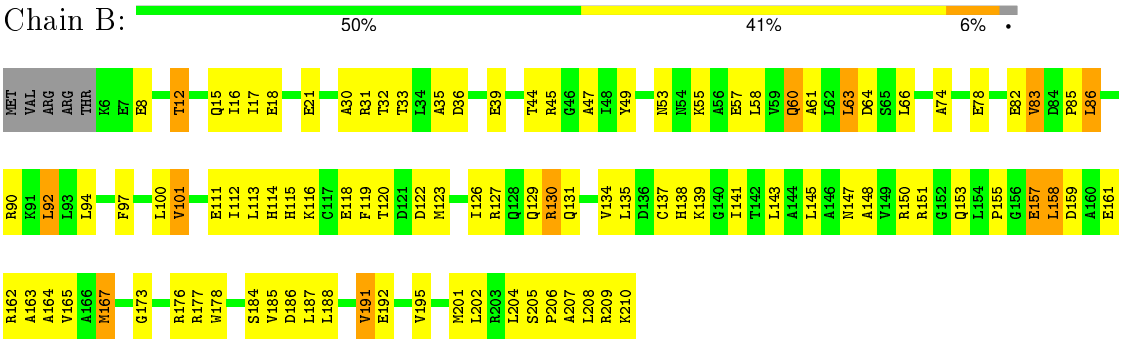
- Molecule 1: HTH-TYPE TRANSCRIPTIONAL REGULATOR TTGR

Chain A:



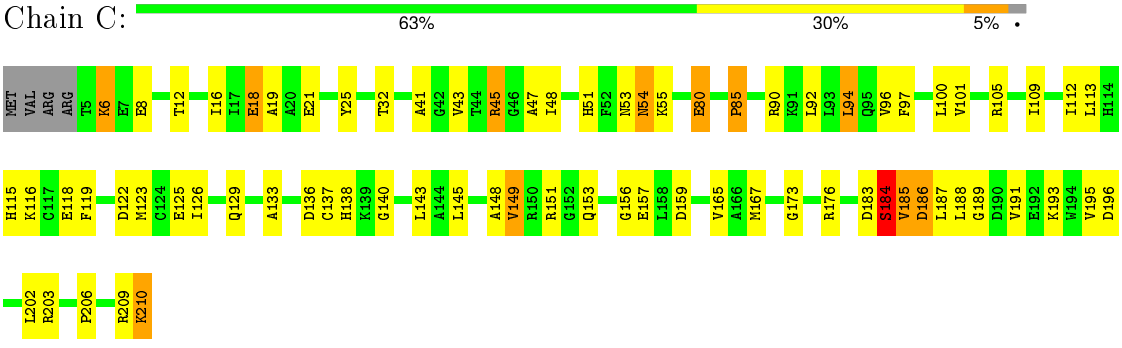
- Molecule 1: HTH-TYPE TRANSCRIPTIONAL REGULATOR TTGR

Chain B:



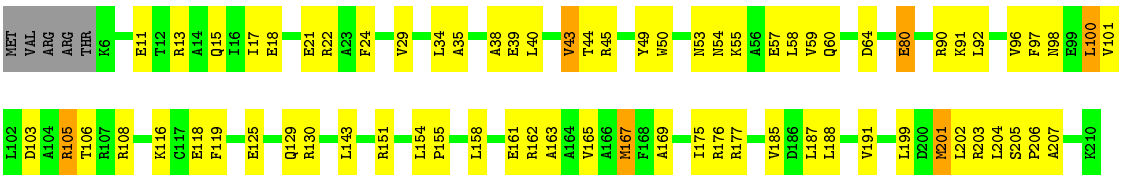
- Molecule 1: HTH-TYPE TRANSCRIPTIONAL REGULATOR TTGR

Chain C:



- Molecule 1: HTH-TYPE TRANSCRIPTIONAL REGULATOR TTGR

Chain D:


MET
VAL
ARG
ARG
THR
K6
E11
T12
R13
A14
Q15
I16
I17
E18
E21
R22
A23
F24
V29
L34
A35
A38
E39
L40
V43
T44
R45
Y49
W50
N53
N54
K55
A56
E57
L58
V59
Q60
D64
E80
R90
K91
L92
V96
F97
N98
E99
L100
V101
L102
D103
A104
R105
T106
R107
R108
K116
C117
E118
F119
E125
Q129
R130
L143
R151
L154
P155
L158
E161
R162
A163
A164
V165
A166
M167
F168
A169
I175
R176
R177
V185
D186
L187
L188
V191
L199
D200
M201
L202
R203
L204
S205
P206
A207
K210

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	43.11Å 43.17Å 114.80Å 96.93° 99.26° 96.03°	Depositor
Resolution (Å)	41.74 – 2.20 42.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.3 (41.74-2.20) 83.1 (42.20-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.218 , 0.288 0.220 , 0.284	Depositor DCC
R_{free} test set	1795 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 22.3	EDS
Estimated twinning fraction	0.067 for k,h,-h-k-l 0.175 for -k,-h,-l 0.058 for -h,-k,h+k+l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 35518 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6363	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.65% 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	0.44	0/1600	0.65	1/2168 (0.0%)
1	B	0.40	0/1603	0.63	0/2172
1	C	0.43	0/1628	0.61	0/2202
1	D	0.43	0/1616	0.60	0/2190
All	All	0.43	0/6447	0.62	1/8732 (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	A	90	ARG	NE-CZ-NH1	-5.39	117.61	120.30

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	1577	0	1541	57	0
1	B	1580	0	1552	82	0
1	C	1605	0	1591	55	0
1	D	1590	0	1565	56	0
2	A	2	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6363	0	6249	227	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 18.

All (227) 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:C:18:GLU:HG3	1:C:105:ARG:HH12	1.25	1.00
1:C:109:ILE:O	1:C:113:LEU:HD23	1.67	0.93
1:C:90:ARG:HH12	1:C:196:ASP:CG	1.77	0.88
1:D:163:ALA:HB1	1:D:202:LEU:HD22	1.57	0.85
1:B:86:LEU:HD13	1:B:153:GLN:HB3	1.56	0.85
1:C:119:PHE:O	1:D:116:LYS:HE2	1.77	0.84
1:B:32:THR:O	1:B:55:LYS:HD2	1.78	0.83
1:D:11:GLU:O	1:D:15:GLN:HG3	1.82	0.80
1:B:86:LEU:HD12	1:B:148:ALA:HB1	1.63	0.80
1:B:44:THR:HG23	1:B:47:ALA:H	1.47	0.80
1:D:21:GLU:OE1	1:D:105:ARG:HD2	1.85	0.77
1:C:18:GLU:HG3	1:C:105:ARG:NH1	1.98	0.77
1:B:83:VAL:HA	1:B:151:ARG:HE	1.50	0.77
1:C:85:PRO:HD2	1:C:153:GLN:OE1	1.85	0.76
1:B:157:GLU:O	1:B:210:LYS:HG3	1.84	0.76
1:C:183:ASP:O	1:C:184:SER:HB2	1.85	0.76
1:A:63:LEU:HB2	1:A:113:LEU:HD11	1.69	0.74
1:A:90:ARG:NH1	1:A:196:ASP:OD1	2.20	0.74
1:C:185:VAL:O	1:C:187:LEU:N	2.20	0.74
1:A:176:ARG:HD3	1:B:176:ARG:CZ	2.18	0.74
1:B:167:MET:HG2	1:B:202:LEU:HD11	1.70	0.73
1:B:201:MET:O	1:B:205:SER:HB3	1.89	0.73
1:C:97:PHE:O	1:C:101:VAL:HG23	1.90	0.71
1:D:101:VAL:HG11	1:D:188:LEU:HB2	1.73	0.71
1:B:111:GLU:OE1	1:B:115:HIS:HD2	1.74	0.70
1:C:112:ILE:HA	1:C:116:LYS:HB2	1.73	0.69
1:B:97:PHE:O	1:B:101:VAL:HG23	1.93	0.69
1:B:147:ASN:HA	1:B:150:ARG:NH1	2.08	0.68
1:B:185:VAL:O	1:B:187:LEU:N	2.26	0.68
1:D:98:ASN:OD1	1:D:191:VAL:HG11	1.94	0.68
1:B:63:LEU:HD23	1:B:64:ASP:N	2.08	0.67
1:A:176:ARG:HD3	1:B:176:ARG:NH1	2.09	0.66
1:D:103:ASP:HB3	1:D:106:THR:HB	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LYS:HD3	1:D:162:ARG:NH2	2.11	0.66
1:C:186:ASP:OD2	1:C:189:GLY:HA3	1.96	0.65
1:C:16:ILE:HD13	1:C:48:ILE:HG13	1.77	0.65
1:B:92:LEU:HD23	1:B:92:LEU:C	2.17	0.65
1:B:33:THR:O	1:B:36:ASP:HB2	1.97	0.65
1:D:125:GLU:O	1:D:129:GLN:HG3	1.97	0.65
1:A:101:VAL:HG11	1:A:188:LEU:HB2	1.79	0.64
1:C:173:GLY:HA3	1:D:169:ALA:O	1.97	0.64
1:A:33:THR:HG22	1:A:36:ASP:CG	2.18	0.64
1:D:38:ALA:HB3	1:D:45:ARG:HG3	1.81	0.63
1:B:147:ASN:HA	1:B:150:ARG:HH12	1.63	0.63
1:D:35:ALA:HB1	1:D:45:ARG:HE	1.64	0.63
1:B:74:ALA:O	1:B:78:GLU:HG3	1.99	0.63
1:A:180:LEU:HD21	1:B:134:VAL:HG21	1.81	0.63
1:B:130:ARG:O	1:B:134:VAL:HG23	1.99	0.62
1:D:167:MET:HG3	1:D:202:LEU:HD11	1.82	0.62
1:C:18:GLU:CG	1:C:105:ARG:HH12	2.06	0.62
1:A:188:LEU:HD12	1:A:188:LEU:O	2.00	0.61
1:A:33:THR:HG22	1:A:36:ASP:OD2	1.99	0.61
1:A:112:ILE:HA	1:A:116:LYS:HB2	1.83	0.61
1:C:206:PRO:HA	1:C:209:ARG:HG2	1.83	0.61
1:B:92:LEU:HD23	1:B:92:LEU:O	2.00	0.60
1:C:92:LEU:HD23	1:C:96:VAL:HG23	1.85	0.59
1:A:119:PHE:O	1:B:116:LYS:HE2	2.02	0.59
1:B:83:VAL:HA	1:B:151:ARG:NE	2.18	0.58
1:B:12:THR:HA	1:B:15:GLN:HG2	1.83	0.58
1:A:60:GLN:HB2	1:A:129:GLN:HG2	1.85	0.58
1:D:53:ASN:HB2	1:D:57:GLU:CD	2.23	0.58
1:A:204:LEU:O	1:A:206:PRO:HD3	2.03	0.58
1:B:101:VAL:HG11	1:B:188:LEU:HB2	1.85	0.57
1:B:86:LEU:HD12	1:B:148:ALA:CB	2.34	0.57
1:A:6:LYS:HE3	1:A:6:LYS:O	2.03	0.57
1:D:167:MET:CG	1:D:202:LEU:HD11	2.34	0.57
1:D:55:LYS:O	1:D:59:VAL:HG23	2.04	0.56
1:C:90:ARG:NH1	1:C:196:ASP:OD1	2.39	0.56
1:D:201:MET:O	1:D:205:SER:HB3	2.05	0.56
1:B:127:ARG:O	1:B:131:GLN:HG3	2.05	0.56
1:A:33:THR:CG2	1:A:36:ASP:H	2.17	0.56
1:D:92:LEU:HD23	1:D:96:VAL:HG23	1.87	0.56
1:C:118:GLU:HG3	1:D:118:GLU:HG3	1.86	0.56
1:A:33:THR:HG23	1:A:36:ASP:H	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLU:OE1	1:B:115:HIS:CD2	2.57	0.55
1:B:12:THR:O	1:B:16:ILE:HG13	2.06	0.55
1:B:63:LEU:C	1:B:63:LEU:HD23	2.27	0.55
1:A:188:LEU:O	1:A:191:VAL:HG22	2.06	0.55
1:C:145:LEU:O	1:C:149:VAL:HG12	2.06	0.55
1:A:180:LEU:CD2	1:B:134:VAL:HG21	2.36	0.55
1:B:60:GLN:HE22	1:B:129:GLN:HG2	1.72	0.55
1:A:21:GLU:OE2	1:A:105:ARG:HD2	2.07	0.54
1:B:60:GLN:NE2	1:B:129:GLN:HG2	2.22	0.54
1:A:186:ASP:OD2	1:A:189:GLY:HA3	2.07	0.54
1:B:159:ASP:CG	1:B:162:ARG:HD3	2.28	0.54
1:A:114:HIS:HE1	1:A:172:ASP:OD1	1.90	0.53
1:A:90:ARG:HH12	1:A:196:ASP:CG	2.11	0.53
1:B:112:ILE:HA	1:B:116:LYS:HB2	1.91	0.53
1:D:22:ARG:HA	1:D:108:ARG:NH2	2.24	0.53
1:D:18:GLU:O	1:D:22:ARG:HG3	2.09	0.53
1:D:35:ALA:O	1:D:39:GLU:HG3	2.09	0.52
1:D:22:ARG:HA	1:D:108:ARG:HH22	1.74	0.52
1:D:45:ARG:O	1:D:49:TYR:CD2	2.61	0.52
1:C:123:MET:HG2	1:C:126:ILE:HG13	1.91	0.52
1:B:90:ARG:NH2	1:B:192:GLU:OE1	2.42	0.52
1:B:177:ARG:NH1	1:B:184:SER:OG	2.42	0.52
1:A:31:ARG:NE	1:B:30:ALA:HB1	2.25	0.52
1:C:92:LEU:HD23	1:C:92:LEU:C	2.30	0.52
1:B:162:ARG:NH2	1:B:207:ALA:O	2.27	0.52
1:A:122:ASP:OD2	1:B:31:ARG:NH2	2.43	0.51
1:C:32:THR:O	1:C:55:LYS:HD2	2.10	0.51
1:B:139:LYS:O	1:B:143:LEU:HG	2.10	0.51
1:D:35:ALA:HA	1:D:45:ARG:HG2	1.92	0.51
1:B:101:VAL:HG11	1:B:188:LEU:CB	2.40	0.51
1:A:137:CYS:O	1:A:141:ILE:HG13	2.11	0.51
1:A:43:VAL:CG1	1:A:47:ALA:HB3	2.40	0.51
1:D:43:VAL:HG23	1:D:44:THR:O	2.10	0.51
1:C:12:THR:HG23	1:C:43:VAL:HG11	1.93	0.50
1:D:92:LEU:HD23	1:D:92:LEU:C	2.32	0.50
1:D:38:ALA:HB3	1:D:45:ARG:CG	2.40	0.50
1:C:210:LYS:HB2	1:C:210:LYS:NZ	2.25	0.50
1:C:125:GLU:O	1:C:129:GLN:HG3	2.11	0.50
1:C:176:ARG:CD	1:D:176:ARG:NH1	2.74	0.50
1:A:169:ALA:O	1:B:173:GLY:HA3	2.12	0.50
1:B:123:MET:HE2	1:B:126:ILE:HD11	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:CYS:O	1:B:141:ILE:HG13	2.12	0.50
1:B:159:ASP:OD2	1:B:162:ARG:HD3	2.11	0.49
1:C:115:HIS:HB3	1:D:119:PHE:CD1	2.47	0.49
1:A:203:ARG:NH1	1:A:204:LEU:HD21	2.26	0.49
1:D:22:ARG:NH2	1:D:40:LEU:HG	2.27	0.49
1:D:13:ARG:O	1:D:17:ILE:HG12	2.12	0.49
1:C:167:MET:HE2	1:C:202:LEU:HD11	1.94	0.49
1:C:90:ARG:NH1	1:C:196:ASP:CG	2.58	0.48
1:B:94:LEU:HD23	1:B:195:VAL:HG21	1.95	0.48
1:A:62:LEU:HD22	1:A:109:ILE:HG12	1.95	0.48
1:D:167:MET:HE3	1:D:199:LEU:HD23	1.94	0.48
1:C:167:MET:HE2	1:C:167:MET:HB2	1.68	0.48
1:A:94:LEU:HD13	1:A:195:VAL:HG21	1.96	0.48
1:D:97:PHE:O	1:D:101:VAL:HG23	2.14	0.48
1:B:158:LEU:CD1	1:B:163:ALA:HB2	2.43	0.48
1:C:138:HIS:HE1	1:C:165:VAL:HG23	1.79	0.48
1:D:154:LEU:O	1:D:155:PRO:C	2.52	0.48
1:B:158:LEU:HD22	1:B:208:LEU:O	2.14	0.47
1:C:21:GLU:OE1	1:C:105:ARG:HD3	2.14	0.47
1:B:58:LEU:O	1:B:61:ALA:HB3	2.13	0.47
1:B:158:LEU:HD11	1:B:163:ALA:HB2	1.96	0.47
1:C:148:ALA:O	1:C:153:GLN:HB2	2.14	0.47
1:B:63:LEU:CD2	1:B:64:ASP:N	2.78	0.47
1:B:82:GLU:O	1:B:85:PRO:HD3	2.16	0.46
1:A:115:HIS:HB3	1:B:119:PHE:CD1	2.50	0.46
1:C:54:ASN:HD22	1:C:54:ASN:C	2.18	0.46
1:C:6:LYS:HG2	1:C:6:LYS:O	2.12	0.46
1:A:84:ASP:CG	1:A:87:GLY:HA3	2.36	0.46
1:D:34:LEU:CD2	1:D:58:LEU:HD12	2.45	0.46
1:C:47:ALA:O	1:C:51:HIS:HD2	1.99	0.46
1:C:157:GLU:O	1:C:210:LYS:N	2.44	0.46
1:B:204:LEU:O	1:B:206:PRO:HD3	2.15	0.46
1:B:92:LEU:CD2	1:B:92:LEU:C	2.84	0.46
1:C:206:PRO:HA	1:C:209:ARG:CG	2.45	0.46
1:D:204:LEU:O	1:D:206:PRO:HD3	2.15	0.45
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.60	0.45
1:B:97:PHE:O	1:B:101:VAL:CG2	2.63	0.45
1:A:115:HIS:O	1:A:116:LYS:HG3	2.17	0.45
1:B:66:LEU:HA	1:B:66:LEU:HD23	1.81	0.45
1:C:159:ASP:HB2	1:C:210:LYS:OXT	2.17	0.45
1:B:53:ASN:ND2	1:B:57:GLU:OE2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ARG:HG3	1:D:199:LEU:HD11	1.99	0.45
1:C:209:ARG:O	1:C:210:LYS:CB	2.64	0.45
1:B:178:TRP:HD1	1:B:185:VAL:HB	1.81	0.45
1:C:149:VAL:HG23	1:C:156:GLY:HA2	1.99	0.45
1:A:192:GLU:H	1:A:192:GLU:HG2	1.41	0.45
1:B:82:GLU:C	1:B:151:ARG:HH21	2.19	0.44
1:B:8:GLU:O	1:B:12:THR:HG23	2.18	0.44
1:C:80:GLU:O	1:C:151:ARG:NH2	2.50	0.44
1:A:49:TYR:CE2	1:C:45:ARG:HG2	2.52	0.44
1:A:119:PHE:CD1	1:B:115:HIS:HB3	2.53	0.44
1:A:78:GLU:O	1:A:143:LEU:HD13	2.17	0.44
1:D:80:GLU:O	1:D:151:ARG:NH2	2.51	0.44
1:A:84:ASP:OD2	1:A:87:GLY:HA3	2.18	0.44
1:C:140:GLY:O	1:C:143:LEU:HB2	2.17	0.44
1:D:143:LEU:HD23	1:D:143:LEU:HA	1.81	0.44
1:B:35:ALA:O	1:B:39:GLU:HG3	2.17	0.44
1:B:141:ILE:O	1:B:145:LEU:HG	2.18	0.43
1:D:35:ALA:HB1	1:D:45:ARG:NE	2.31	0.43
1:B:111:GLU:OE1	1:B:111:GLU:HA	2.19	0.43
1:A:188:LEU:HD12	1:A:188:LEU:C	2.38	0.43
1:D:188:LEU:HA	1:D:191:VAL:HG13	2.01	0.43
1:D:162:ARG:NH2	1:D:207:ALA:O	2.50	0.43
1:A:125:GLU:O	1:A:129:GLN:HB2	2.18	0.43
1:D:34:LEU:HD23	1:D:58:LEU:HD12	2.00	0.43
1:D:167:MET:CE	1:D:199:LEU:HD23	2.49	0.43
1:C:25:TYR:HB2	1:C:112:ILE:HD11	2.01	0.43
1:B:120:THR:O	1:B:123:MET:N	2.42	0.43
1:B:123:MET:CE	1:B:126:ILE:HD11	2.48	0.43
1:B:188:LEU:O	1:B:188:LEU:HD12	2.19	0.43
1:A:154:LEU:HA	1:A:154:LEU:HD23	1.88	0.42
1:B:113:LEU:O	1:B:130:ARG:NH2	2.52	0.42
1:D:161:GLU:O	1:D:165:VAL:HG23	2.20	0.42
1:D:53:ASN:HB2	1:D:57:GLU:OE2	2.19	0.42
1:B:45:ARG:O	1:B:49:TYR:HD1	2.02	0.42
1:A:31:ARG:HE	1:B:30:ALA:HB1	1.84	0.42
1:A:43:VAL:HG12	1:A:47:ALA:HB3	2.01	0.42
1:A:176:ARG:HH22	1:B:114:HIS:HA	1.85	0.42
1:C:101:VAL:HG11	1:C:188:LEU:HB2	2.01	0.42
1:A:21:GLU:OE2	1:A:108:ARG:NH1	2.52	0.42
1:A:100:LEU:HD11	1:A:175:ILE:HG23	2.01	0.42
1:A:33:THR:HG23	1:A:35:ALA:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:O	1:A:151:ARG:NH2	2.53	0.42
1:B:17:ILE:O	1:B:21:GLU:HG3	2.19	0.42
1:A:176:ARG:NH1	1:B:176:ARG:CD	2.83	0.42
1:D:50:TRP:O	1:D:50:TRP:CD1	2.73	0.42
1:A:79:SER:O	1:A:82:GLU:HB3	2.20	0.42
1:D:100:LEU:HD11	1:D:175:ILE:HG23	2.02	0.42
1:C:94:LEU:HD13	1:C:195:VAL:HG21	2.02	0.42
1:A:118:GLU:HG3	1:B:118:GLU:HG3	2.02	0.41
1:D:64:ASP:OD1	1:D:64:ASP:N	2.53	0.41
1:A:103:ASP:HB3	1:A:106:THR:HB	2.01	0.41
1:C:183:ASP:O	1:C:184:SER:CB	2.60	0.41
1:B:188:LEU:HA	1:B:191:VAL:HG22	2.02	0.41
1:D:38:ALA:CB	1:D:45:ARG:HG3	2.50	0.41
1:C:138:HIS:CE1	1:C:165:VAL:HG23	2.56	0.41
1:A:49:TYR:CZ	1:C:45:ARG:HG2	2.55	0.41
1:A:6:LYS:HE3	1:A:6:LYS:C	2.41	0.41
1:C:19:ALA:HB3	1:C:41:ALA:HB2	2.02	0.41
1:B:155:PRO:HG2	1:B:209:ARG:HE	1.86	0.41
1:D:187:LEU:O	1:D:191:VAL:CG1	2.69	0.41
1:B:138:HIS:CE1	1:B:164:ALA:HB3	2.55	0.41
1:C:133:ALA:O	1:C:137:CYS:HB2	2.21	0.41
1:B:161:GLU:O	1:B:165:VAL:HG23	2.21	0.41
1:A:90:ARG:HD2	1:A:90:ARG:HH11	1.72	0.40
1:D:187:LEU:O	1:D:191:VAL:HG13	2.20	0.40
1:C:85:PRO:HG2	1:C:148:ALA:HA	2.02	0.40
1:A:5:THR:O	1:A:6:LYS:HB3	2.21	0.40
1:C:165:VAL:HG11	1:D:185:VAL:HG22	2.02	0.40
1:D:24:PHE:CD2	1:D:29:VAL:HA	2.56	0.40
1:D:154:LEU:HB3	1:D:155:PRO:HD2	2.03	0.40
1:B:45:ARG:HE	1:B:45:ARG:HB2	1.77	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	204/210 (97%)	190 (93%)	12 (6%)	2 (1%)	19 16
1	B	203/210 (97%)	192 (95%)	10 (5%)	1 (0%)	34 35
1	C	204/210 (97%)	189 (93%)	12 (6%)	3 (2%)	13 9
1	D	204/210 (97%)	193 (95%)	11 (5%)	0	100 100
All	All	815/840 (97%)	764 (94%)	45 (6%)	6 (1%)	26 25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	184	SER
1	C	186	ASP
1	A	45	ARG
1	A	6	LYS
1	B	186	ASP
1	C	185	VAL

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	157/174 (90%)	138 (88%)	19 (12%)	6 5
1	B	157/174 (90%)	141 (90%)	16 (10%)	9 8
1	C	163/174 (94%)	146 (90%)	17 (10%)	9 8
1	D	160/174 (92%)	147 (92%)	13 (8%)	15 14
All	All	637/696 (92%)	572 (90%)	65 (10%)	9 8

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	18	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	80	GLU
1	A	89	MET
1	A	94	LEU
1	A	100	LEU
1	A	105	ARG
1	A	108	ARG
1	A	121	ASP
1	A	123	MET
1	A	124	CYS
1	A	129	GLN
1	A	130	ARG
1	A	143	LEU
1	A	167	MET
1	A	177	ARG
1	A	191	VAL
1	A	192	GLU
1	A	203	ARG
1	B	12	THR
1	B	18	GLU
1	B	60	GLN
1	B	63	LEU
1	B	83	VAL
1	B	86	LEU
1	B	92	LEU
1	B	100	LEU
1	B	101	VAL
1	B	122	ASP
1	B	130	ARG
1	B	135	LEU
1	B	157	GLU
1	B	158	LEU
1	B	167	MET
1	B	191	VAL
1	C	6	LYS
1	C	8	GLU
1	C	18	GLU
1	C	45	ARG
1	C	53	ASN
1	C	54	ASN
1	C	80	GLU
1	C	85	PRO
1	C	94	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	100	LEU
1	C	122	ASP
1	C	136	ASP
1	C	149	VAL
1	C	184	SER
1	C	191	VAL
1	C	203	ARG
1	C	210	LYS
1	D	43	VAL
1	D	54	ASN
1	D	60	GLN
1	D	80	GLU
1	D	91	LYS
1	D	100	LEU
1	D	105	ARG
1	D	130	ARG
1	D	158	LEU
1	D	167	MET
1	D	177	ARG
1	D	201	MET
1	D	203	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	95	GLN
1	A	110	ASN
1	A	114	HIS
1	A	115	HIS
1	B	60	GLN
1	B	95	GLN
1	B	110	ASN
1	B	115	HIS
1	B	138	HIS
1	C	51	HIS
1	C	54	ASN
1	C	110	ASN
1	C	114	HIS
1	C	115	HIS
1	C	129	GLN
1	D	15	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	110	ASN
1	D	115	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	206/210 (98%)	-0.56	0	100	100	19, 32, 51, 75	0
1	B	205/210 (97%)	-0.50	0	100	100	21, 34, 49, 54	0
1	C	206/210 (98%)	-0.49	0	100	100	22, 35, 48, 64	0
1	D	205/210 (97%)	-0.51	0	100	100	21, 32, 50, 60	0
All	All	822/840 (97%)	-0.52	0	100	100	19, 33, 50, 75	0

There are no RSRZ outliers to report.

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.