



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:53 PM GMT

PDB ID : 4GK0
Title : Crystal structure of human Rev3-Rev7-Rev1 complex
Authors : Tao, J.; Min, X.; Wei, X.
Deposited on : 2012-08-10
Resolution : 2.70 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

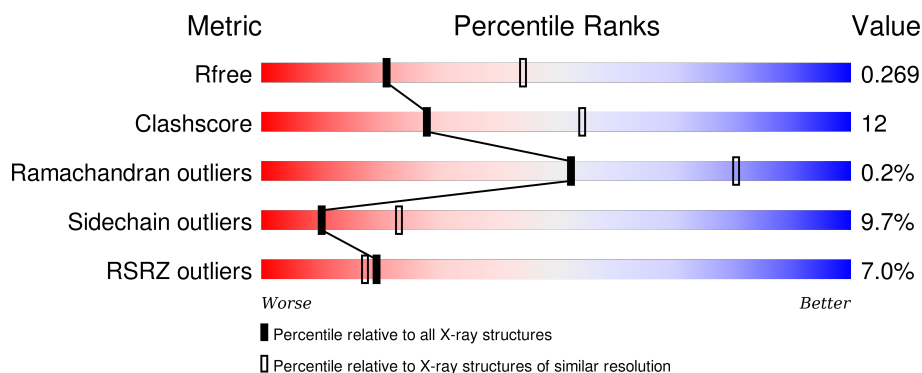
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 $\leq 5\%$. 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	238	<div> <div>4%</div> <div>61% 18% 17%</div> </div>
1	B	238	<div> <div>5%</div> <div>58% 18% 20%</div> </div>
2	C	52	<div> <div>2%</div> <div>21% 15% 62%</div> </div>
2	D	52	<div> <div>6%</div> <div>21% 17% 62%</div> </div>
3	E	136	<div> <div>3%</div> <div>52% 17% 29%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	136	<div><div></div><div>10%</div><div>43%</div><div>22%</div><div>•</div><div>32%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4987 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 Mitotic spindle assembly checkpoint protein MAD2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1605	1037	270	288	10			
1	B	190	Total	C	N	O	S	0	0	0
			1546	999	261	276	10			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	EXPRESSION TAG	UNP Q9UI95
A	-14	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	-13	SER	-	EXPRESSION TAG	UNP Q9UI95
A	-12	SER	-	EXPRESSION TAG	UNP Q9UI95
A	-11	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-10	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-9	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-8	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-7	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-6	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-5	SER	-	EXPRESSION TAG	UNP Q9UI95
A	-4	GLN	-	EXPRESSION TAG	UNP Q9UI95
A	-3	ASP	-	EXPRESSION TAG	UNP Q9UI95
A	-2	PRO	-	EXPRESSION TAG	UNP Q9UI95
A	-1	ASN	-	EXPRESSION TAG	UNP Q9UI95
A	0	SER	-	EXPRESSION TAG	UNP Q9UI95
A	124	ALA	ARG	ENGINEERED MUTATION	UNP Q9UI95
A	212	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	213	SER	-	EXPRESSION TAG	UNP Q9UI95
A	214	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	215	SER	-	EXPRESSION TAG	UNP Q9UI95
A	216	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	217	SER	-	EXPRESSION TAG	UNP Q9UI95
A	218	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	219	SER	-	EXPRESSION TAG	UNP Q9UI95

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Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	221	SER	-	EXPRESSION TAG	UNP Q9UI95
A	222	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-15	MET	-	EXPRESSION TAG	UNP Q9UI95
B	-14	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	-13	SER	-	EXPRESSION TAG	UNP Q9UI95
B	-12	SER	-	EXPRESSION TAG	UNP Q9UI95
B	-11	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-10	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-9	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-8	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-7	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-6	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-5	SER	-	EXPRESSION TAG	UNP Q9UI95
B	-4	GLN	-	EXPRESSION TAG	UNP Q9UI95
B	-3	ASP	-	EXPRESSION TAG	UNP Q9UI95
B	-2	PRO	-	EXPRESSION TAG	UNP Q9UI95
B	-1	ASN	-	EXPRESSION TAG	UNP Q9UI95
B	0	SER	-	EXPRESSION TAG	UNP Q9UI95
B	124	ALA	ARG	ENGINEERED MUTATION	UNP Q9UI95
B	212	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	213	SER	-	EXPRESSION TAG	UNP Q9UI95
B	214	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	215	SER	-	EXPRESSION TAG	UNP Q9UI95
B	216	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	217	SER	-	EXPRESSION TAG	UNP Q9UI95
B	218	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	219	SER	-	EXPRESSION TAG	UNP Q9UI95
B	220	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	221	SER	-	EXPRESSION TAG	UNP Q9UI95
B	222	HIS	-	EXPRESSION TAG	UNP Q9UI95

- Molecule 2 is a protein called DNA polymerase zeta catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	S	0	0	0
			151	95	25	29	2			
2	D	20	Total	C	N	O	S	0	0	0
			151	95	25	29	2			

- Molecule 3 is a protein called DNA repair protein REV1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	96	Total	C	N	O	S	0	0	0
			778	500	121	152	5			
3	F	93	Total	C	N	O	S	0	0	0
			756	487	118	146	5			

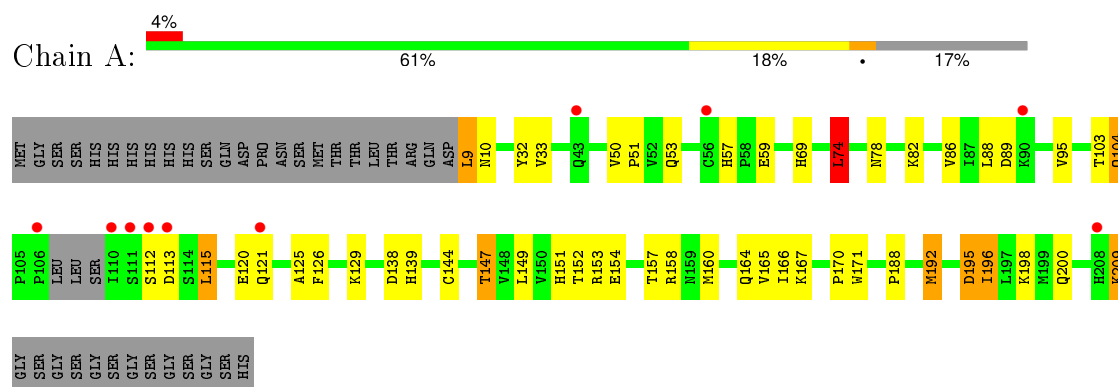
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1116	MET	-	EXPRESSION TAG	UNP Q9UBZ9
F	1116	MET	-	EXPRESSION TAG	UNP Q9UBZ9

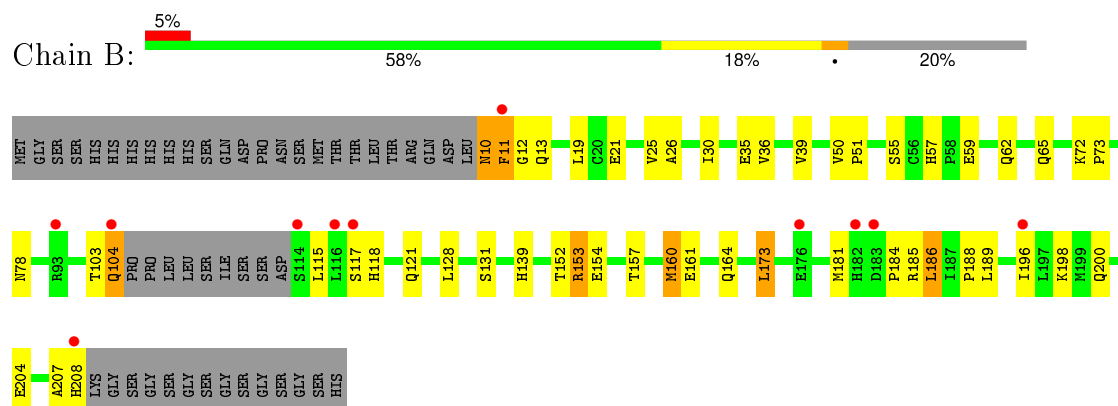
3 Residue-property plots [i](#)

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.

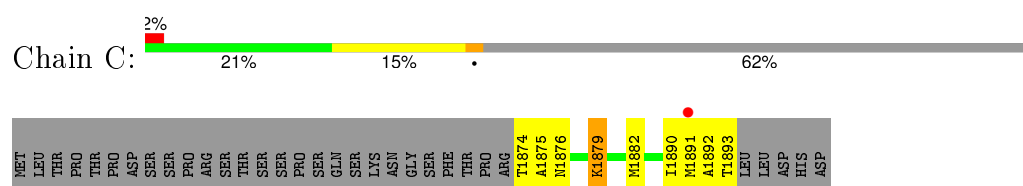
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2B



- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2B

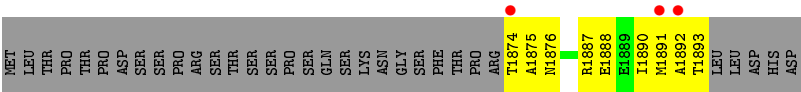


- Molecule 2: DNA polymerase zeta catalytic subunit

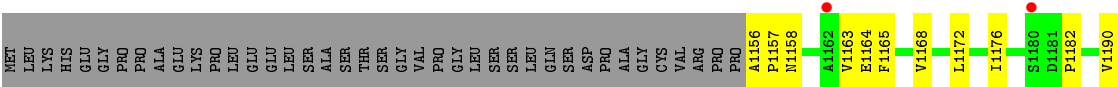


- Molecule 2: DNA polymerase zeta catalytic subunit

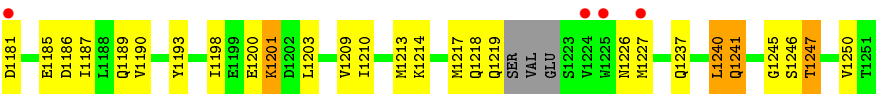
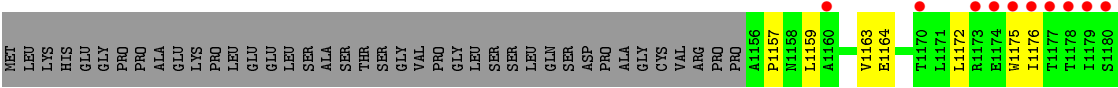
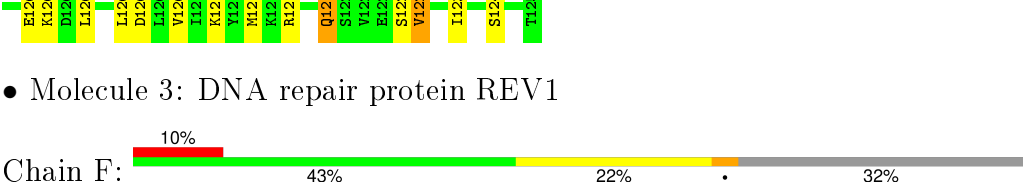




● Molecule 3: DNA repair protein REV1



● Molecule 3: DNA repair protein REV1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.09Å 71.89Å 106.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 35.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-2.70) 95.6 (35.19-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.218 , 0.273 0.214 , 0.269	Depositor DCC
R_{free} test set	1269 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25124 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4987	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.61	0/1640	0.83	1/2228 (0.0%)
1	B	0.50	0/1579	0.70	0/2144
2	C	0.57	0/153	0.81	0/207
2	D	0.54	0/153	0.75	0/207
3	E	0.64	0/789	0.83	0/1070
3	F	0.49	0/766	0.72	0/1037
All	All	0.56	0/5080	0.77	1/6893 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1605	0	1640	35	0
1	B	1546	0	1577	42	0
2	C	151	0	160	7	0
2	D	151	0	160	8	0
3	E	778	0	789	20	0
3	F	756	0	768	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4987	0	5094	118	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 12.

All (118) 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:153:ARG:HG3	1:B:153:ARG:HH11	1.25	0.99
1:B:207:ALA:O	1:B:208:HIS:HB3	1.70	0.92
3:E:1172:LEU:HD13	3:E:1213:MET:CE	2.07	0.83
2:C:1874:THR:OG1	2:C:1875:ALA:N	2.12	0.82
3:F:1237:GLN:HG3	3:F:1247:THR:HG22	1.69	0.74
1:A:9:LEU:HD12	1:A:104:GLN:CB	2.18	0.73
1:A:9:LEU:HD12	1:A:104:GLN:HB3	1.72	0.72
1:B:153:ARG:HH11	1:B:153:ARG:CG	2.04	0.70
3:F:1237:GLN:NE2	3:F:1247:THR:HB	2.07	0.70
1:B:200:GLN:NE2	3:F:1203:LEU:H	1.89	0.70
3:F:1172:LEU:O	3:F:1176:ILE:HG13	1.95	0.66
1:A:200:GLN:NE2	3:E:1203:LEU:H	1.95	0.65
3:F:1237:GLN:HE21	3:F:1247:THR:HB	1.62	0.64
1:A:9:LEU:HD22	1:A:10:ASN:N	2.13	0.64
3:F:1214:LYS:O	3:F:1218:GLN:HG3	1.97	0.63
3:F:1175:TRP:CZ2	3:F:1186:ASP:HB3	2.34	0.63
1:B:11:PHE:HD2	1:B:12:GLY:H	1.42	0.63
1:A:69:HIS:HD2	1:A:166:ILE:HD11	1.64	0.63
1:A:50:VAL:HB	1:A:51:PRO:HD2	1.80	0.62
1:A:57:HIS:CD2	2:C:1890:ILE:HD13	2.34	0.62
1:B:153:ARG:HG3	1:B:153:ARG:NH1	2.02	0.62
1:B:200:GLN:HE21	3:F:1203:LEU:H	1.47	0.62
2:D:1888:GLU:H	2:D:1888:GLU:CD	2.03	0.62
3:F:1213:MET:O	3:F:1217:MET:HB2	2.00	0.62
3:E:1172:LEU:CD1	3:E:1213:MET:CE	2.78	0.61
1:A:138:ASP:HB2	1:A:209:LYS:HE2	1.82	0.61
1:A:188:PRO:HG2	3:E:1207:ASP:HB2	1.83	0.60
1:A:164:GLN:HE22	1:A:171:TRP:H	1.49	0.60
1:B:57:HIS:CD2	2:D:1890:ILE:HG23	2.37	0.60
3:E:1172:LEU:HD13	3:E:1213:MET:HE2	1.82	0.60
1:B:103:THR:O	1:B:198:LYS:HB3	2.02	0.59
1:B:57:HIS:CE1	1:B:59:GLU:HB3	2.37	0.59
3:F:1218:GLN:O	3:F:1219:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:GLN:HE22	3:F:1203:LEU:HG	1.68	0.59
1:A:149:LEU:HD23	2:C:1879:LYS:HB2	1.84	0.59
1:A:86:VAL:HB	1:A:147:THR:HG23	1.84	0.59
1:A:89:ASP:C	1:A:89:ASP:OD1	2.40	0.58
1:B:160:MET:HE1	1:B:173:LEU:HD12	1.84	0.58
3:E:1156:ALA:N	3:E:1157:PRO:CD	2.67	0.58
1:A:9:LEU:HD22	1:A:10:ASN:H	1.69	0.58
1:B:153:ARG:CG	1:B:153:ARG:NH1	2.65	0.57
1:A:103:THR:HG22	1:A:104:GLN:N	2.20	0.57
1:B:50:VAL:HB	1:B:51:PRO:HD2	1.87	0.56
1:B:160:MET:CE	1:B:173:LEU:HD12	2.36	0.56
1:A:195:ASP:HB3	1:A:196:ILE:HG23	1.86	0.56
1:B:157:THR:O	1:B:161:GLU:HG3	2.06	0.55
1:B:10:ASN:N	1:B:10:ASN:OD1	2.38	0.55
2:D:1890:ILE:C	2:D:1892:ALA:H	2.10	0.55
1:A:78:ASN:O	1:A:153:ARG:HD2	2.06	0.55
2:C:1874:THR:HG1	2:C:1875:ALA:H	1.51	0.54
1:B:26:ALA:O	1:B:30:ILE:HG13	2.08	0.53
1:A:82:LYS:HB2	1:A:151:HIS:HB2	1.91	0.53
1:B:207:ALA:O	1:B:208:HIS:CB	2.48	0.52
3:F:1157:PRO:HG3	3:F:1200:GLU:HG3	1.91	0.51
1:A:164:GLN:HE22	1:A:171:TRP:N	2.08	0.51
1:A:152:THR:OG1	2:C:1876:ASN:HB2	2.11	0.51
1:B:188:PRO:O	1:B:189:LEU:HD23	2.11	0.51
1:A:160:MET:O	1:A:164:GLN:HB2	2.10	0.51
1:B:72:LYS:HB3	1:B:73:PRO:HD3	1.92	0.51
3:E:1190:VAL:HG11	3:E:1232:ILE:HD13	1.92	0.51
1:B:11:PHE:CD2	1:B:11:PHE:N	2.77	0.50
1:B:157:THR:HG22	1:B:161:GLU:OE1	2.11	0.50
1:A:125:ALA:O	1:A:129:LYS:HG2	2.11	0.50
3:E:1172:LEU:CD1	3:E:1213:MET:HE1	2.41	0.50
3:F:1163:VAL:HG12	3:F:1164:GLU:N	2.27	0.49
1:A:103:THR:CG2	1:A:104:GLN:N	2.75	0.49
1:B:152:THR:OG1	2:D:1876:ASN:HB2	2.13	0.49
3:F:1175:TRP:HZ2	3:F:1186:ASP:HB3	1.74	0.48
3:E:1158:ASN:HB3	3:E:1163:VAL:HG22	1.96	0.48
1:A:33:VAL:O	1:A:33:VAL:HG12	2.14	0.48
1:A:200:GLN:HE22	3:E:1203:LEU:H	1.62	0.48
3:E:1182:PRO:HD2	3:E:1224:VAL:HG11	1.96	0.48
1:B:78:ASN:O	1:B:153:ARG:NH1	2.48	0.47
1:B:128:LEU:O	1:B:131:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:HIS:HA	1:B:121:GLN:HE21	1.78	0.47
3:E:1156:ALA:HB3	3:E:1157:PRO:HD3	1.96	0.46
1:B:78:ASN:HB2	1:B:104:GLN:NE2	2.30	0.46
3:F:1187:ILE:O	3:F:1190:VAL:HB	2.15	0.46
3:E:1165:PHE:HE1	3:E:1209:VAL:HG23	1.80	0.46
1:A:113:ASP:O	1:A:195:ASP:N	2.48	0.46
1:B:36:VAL:O	2:D:1887:ARG:NH1	2.49	0.46
2:D:1890:ILE:C	2:D:1892:ALA:N	2.69	0.45
1:B:19:LEU:HA	1:B:19:LEU:HD23	1.79	0.45
1:B:185:ARG:O	1:B:204:GLU:HA	2.16	0.45
1:B:35:GLU:OE1	1:B:139:HIS:CE1	2.70	0.45
1:A:120:GLU:N	1:A:120:GLU:OE1	2.43	0.45
1:A:32:TYR:CZ	1:A:53:GLN:HG3	2.51	0.45
1:B:200:GLN:NE2	3:F:1201:LYS:O	2.50	0.44
1:A:115:LEU:H	1:A:195:ASP:HB2	1.83	0.44
3:F:1241:GLN:HG2	3:F:1247:THR:HG23	1.99	0.44
1:B:184:PRO:HG2	3:F:1246:SER:HB3	1.99	0.43
3:E:1165:PHE:O	3:E:1168:VAL:HB	2.18	0.43
3:F:1198:ILE:HD13	3:F:1240:LEU:HD13	2.00	0.43
1:A:198:LYS:HE2	3:E:1201:LYS:HB2	1.99	0.43
2:D:1887:ARG:O	2:D:1891:MET:HG3	2.18	0.43
3:E:1176:ILE:HG22	3:E:1176:ILE:O	2.18	0.43
3:E:1164:GLU:O	3:E:1165:PHE:C	2.56	0.43
1:A:9:LEU:CD1	1:A:104:GLN:CB	2.93	0.43
2:C:1890:ILE:O	2:C:1892:ALA:N	2.52	0.42
1:B:10:ASN:HB3	1:B:13:GLN:HB3	2.01	0.42
1:A:164:GLN:NE2	1:A:170:PRO:HA	2.34	0.42
3:F:1159:LEU:HD13	3:F:1193:TYR:HB2	2.02	0.42
3:E:1207:ASP:OD1	3:E:1211:LYS:HE3	2.19	0.42
1:A:88:LEU:O	1:A:144:CYS:HA	2.20	0.42
1:A:74:LEU:N	1:A:74:LEU:HD23	2.35	0.42
1:B:11:PHE:CD2	1:B:12:GLY:N	2.81	0.42
1:B:186:LEU:HD11	3:F:1203:LEU:HD13	2.01	0.41
1:B:103:THR:O	1:B:103:THR:HG22	2.20	0.41
1:B:160:MET:CE	1:B:173:LEU:CD1	2.98	0.41
3:E:1215:ARG:O	3:E:1219:GLN:HB3	2.20	0.41
3:E:1206:LEU:HD12	3:E:1207:ASP:N	2.36	0.41
3:F:1241:GLN:O	3:F:1245:GLY:HA2	2.21	0.41
1:B:181:MET:HE1	1:B:204:GLU:HB3	2.03	0.41
1:A:126:PHE:HE1	1:A:192:MET:HG2	1.86	0.41
1:B:21:GLU:O	1:B:25:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:HIS:HD2	1:B:121:GLN:NE2	2.18	0.40
2:D:1874:THR:OG1	2:D:1875:ALA:N	2.53	0.40
2:C:1874:THR:HG23	2:C:1876:ASN:OD1	2.21	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	194/238 (82%)	186 (96%)	8 (4%)	0	100	100
1	B	186/238 (78%)	172 (92%)	14 (8%)	0	100	100
2	C	18/52 (35%)	14 (78%)	4 (22%)	0	100	100
2	D	18/52 (35%)	14 (78%)	4 (22%)	0	100	100
3	E	94/136 (69%)	89 (95%)	5 (5%)	0	100	100
3	F	89/136 (65%)	77 (86%)	11 (12%)	1 (1%)	17	42
All	All	599/852 (70%)	552 (92%)	46 (8%)	1 (0%)	52	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	1250	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	186/219 (85%)	167 (90%)	19 (10%)	9	21
1	B	178/219 (81%)	162 (91%)	16 (9%)	12	27
2	C	18/49 (37%)	14 (78%)	4 (22%)	1	3
2	D	18/49 (37%)	17 (94%)	1 (6%)	26	54
3	E	90/123 (73%)	85 (94%)	5 (6%)	26	54
3	F	87/123 (71%)	76 (87%)	11 (13%)	5	13
All	All	577/782 (74%)	521 (90%)	56 (10%)	10	23

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	59	GLU
1	A	74	LEU
1	A	95	VAL
1	A	104	GLN
1	A	112	SER
1	A	115	LEU
1	A	121	GLN
1	A	139	HIS
1	A	147	THR
1	A	154	GLU
1	A	157	THR
1	A	158	ARG
1	A	165	VAL
1	A	167	LYS
1	A	192	MET
1	A	195	ASP
1	A	196	ILE
1	A	209	LYS
1	B	10	ASN
1	B	11	PHE
1	B	39	VAL
1	B	55	SER
1	B	62	GLN
1	B	65	GLN
1	B	104	GLN
1	B	115	LEU
1	B	117	SER
1	B	153	ARG
1	B	154	GLU

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Mol	Chain	Res	Type
1	B	160	MET
1	B	164	GLN
1	B	173	LEU
1	B	186	LEU
1	B	196	ILE
2	C	1879	LYS
2	C	1882	MET
2	C	1891	MET
2	C	1893	THR
2	D	1893	THR
3	E	1200	GLU
3	E	1219	GLN
3	E	1223	SER
3	E	1224	VAL
3	E	1246	SER
3	F	1181	ASP
3	F	1185	GLU
3	F	1189	GLN
3	F	1201	LYS
3	F	1209	VAL
3	F	1210	ILE
3	F	1226	ASN
3	F	1227	MET
3	F	1240	LEU
3	F	1241	GLN
3	F	1247	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	164	GLN
1	A	200	GLN
1	B	10	ASN
1	B	104	GLN
1	B	118	HIS
1	B	121	GLN
1	B	139	HIS
1	B	200	GLN
1	B	208	HIS
3	F	1237	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

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, 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	198/238 (83%)	0.06	10 (5%) 32 30	26, 41, 63, 76	0
1	B	190/238 (79%)	0.16	11 (5%) 26 25	38, 59, 76, 80	0
2	C	20/52 (38%)	0.38	1 (5%) 32 31	32, 50, 81, 82	0
2	D	20/52 (38%)	0.54	3 (15%) 3 2	45, 63, 78, 79	0
3	E	96/136 (70%)	-0.02	4 (4%) 40 39	26, 44, 65, 71	0
3	F	93/136 (68%)	0.78	14 (15%) 3 2	47, 68, 80, 81	0
All	All	617/852 (72%)	0.22	43 (6%) 19 17	26, 53, 76, 82	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1178	THR	5.8
3	F	1160	ALA	5.6
3	F	1179	ILE	4.7
3	E	1221	VAL	3.9
2	C	1891	MET	3.7
1	A	110	ILE	3.6
3	F	1181	ASP	3.5
1	B	93	ARG	3.4
1	A	208	HIS	3.4
1	A	106	PRO	3.3
3	F	1173	ARG	3.3
3	F	1175	TRP	3.3
3	F	1224	VAL	3.1
2	D	1874	THR	3.1
1	B	104	GLN	3.0
3	F	1177	THR	3.0
1	B	196	ILE	3.0
1	A	43	GLN	3.0
3	F	1225	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	112	SER	2.8
3	F	1174	GLU	2.8
2	D	1891	MET	2.7
3	E	1180	SER	2.7
3	F	1180	SER	2.7
1	A	113	ASP	2.5
3	F	1227	MET	2.4
3	F	1170	THR	2.4
1	A	90	LYS	2.4
2	D	1892	ALA	2.4
1	A	111	SER	2.3
1	B	11	PHE	2.3
1	B	114	SER	2.3
3	F	1176	ILE	2.3
1	B	182	HIS	2.2
1	A	121	GLN	2.2
1	B	176	GLU	2.2
1	B	208	HIS	2.1
1	B	117	SER	2.1
1	B	183	ASP	2.1
1	A	56	CYS	2.1
3	E	1251	THR	2.0
1	B	116	LEU	2.0
3	E	1162	ALA	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.