



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:51 pm BST

PDB ID : 5B6M
Title : Crystal structure of human peroxiredoxin 6 in reduced state
Authors : Kim, K.H.; Lee, W.T.; Kim, E.E.
Deposited on : 2016-05-30
Resolution : 2.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

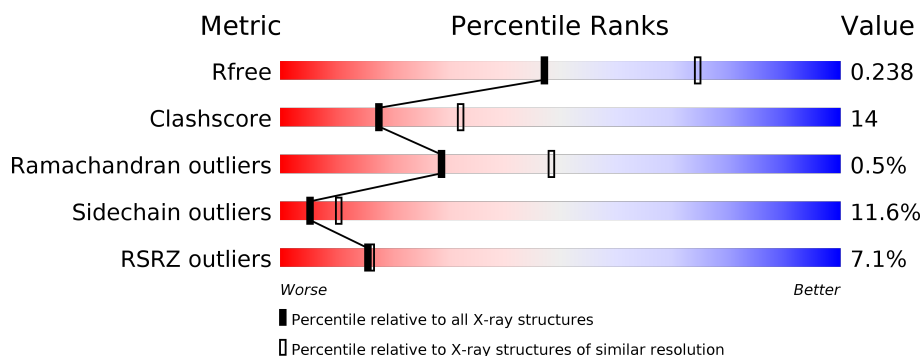
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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 $\leq 5\%$. 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	224	<div> <div></div> <div>75% 21% ..</div> </div>
1	B	224	<div> <div>2%</div> <div>73% 21% 5% .</div> </div>
1	C	224	<div> <div>8%</div> <div>65% 25% 5% .</div> </div>
1	D	224	<div> <div>24%</div> <div>46% 38% 10% 6%</div> </div>
1	E	224	<div> <div>7%</div> <div>51% 40% 6% ..</div> </div>
1	F	224	<div> <div>%</div> <div>67% 27% 5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10485 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 Peroxiredoxin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1747	1127	293	322	5			
1	B	221	Total	C	N	O	S	0	0	0
			1747	1127	293	322	5			
1	C	214	Total	C	N	O	S	0	0	0
			1692	1090	284	313	5			
1	D	211	Total	C	N	O	S	0	0	0
			1670	1081	280	305	4			
1	E	221	Total	C	N	O	S	0	0	0
			1747	1127	293	322	5			
1	F	223	Total	C	N	O	S	0	0	0
			1758	1134	295	324	5			

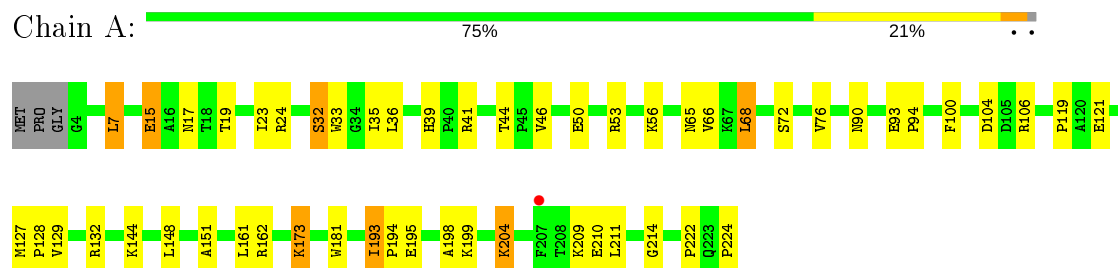
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	31	Total	O	0	0
			31	31		
2	C	18	Total	O	0	0
			18	18		
2	D	10	Total	O	0	0
			10	10		
2	E	20	Total	O	0	0
			20	20		
2	F	22	Total	O	0	0
			22	22		

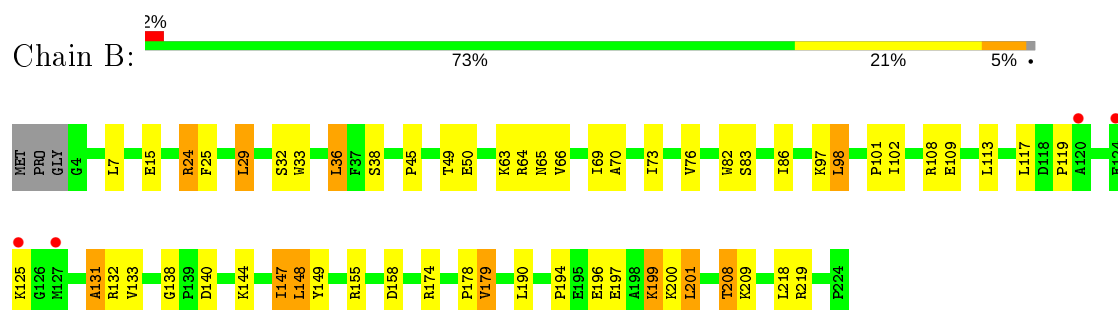
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

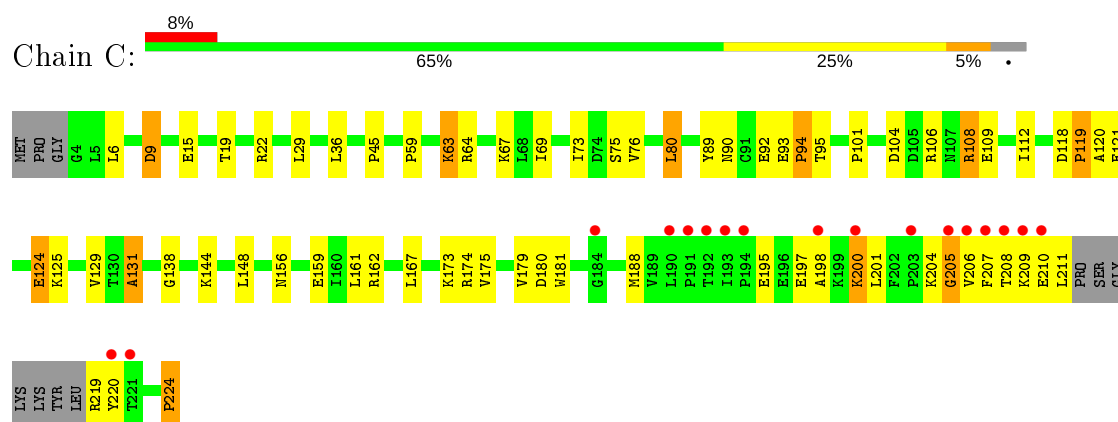
• Molecule 1: Peroxiredoxin-6



• Molecule 1: Peroxiredoxin-6

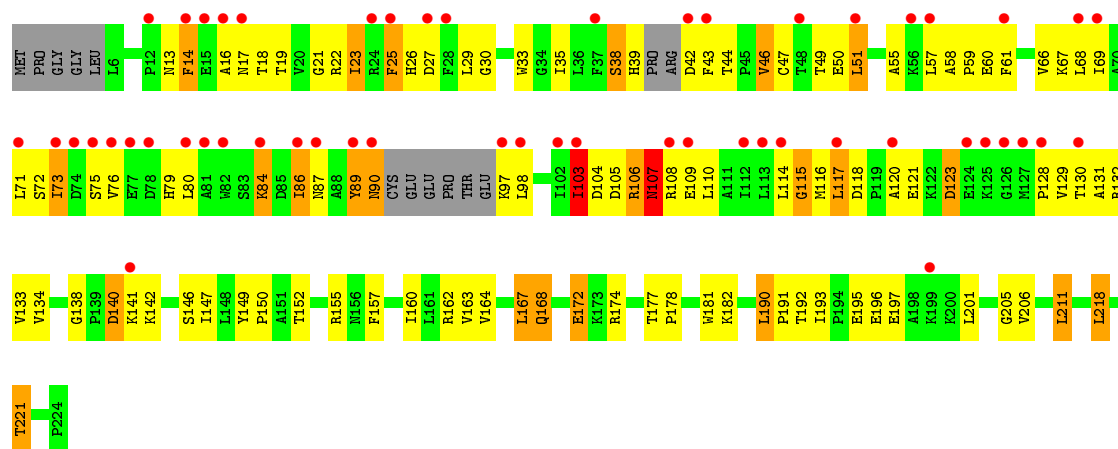


• Molecule 1: Peroxiredoxin-6

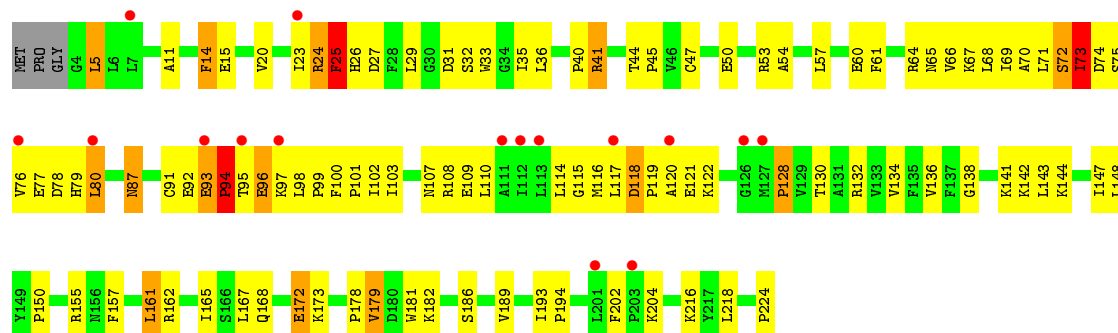


• Molecule 1: Peroxiredoxin-6

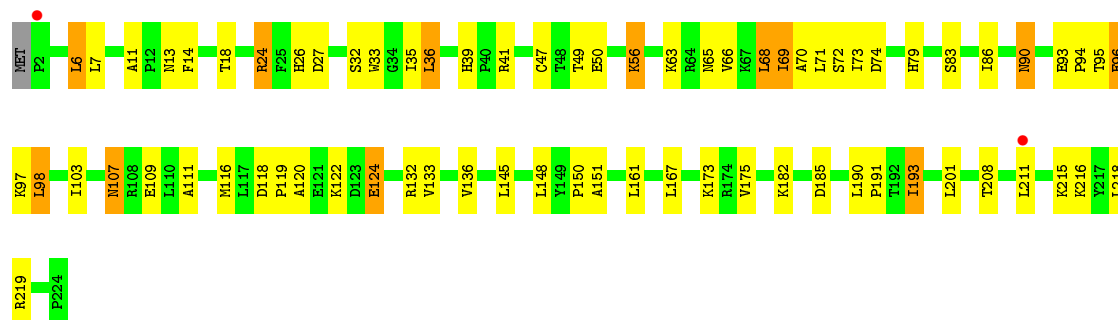




• Molecule 1: Peroxiredoxin-6



• Molecule 1: Peroxiredoxin-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.35Å 106.35Å 165.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.89 – 2.50 48.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (37.89-2.50) 98.7 (48.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.233 , 0.290 0.237 , 0.238	Depositor DCC
R_{free} test set	2926 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10485	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.47	0/1789	0.64	0/2428
1	B	0.49	0/1789	0.70	2/2428 (0.1%)
1	C	0.48	1/1731 (0.1%)	0.84	10/2349 (0.4%)
1	D	0.38	0/1708	0.99	21/2314 (0.9%)
1	E	0.54	1/1789 (0.1%)	0.94	12/2428 (0.5%)
1	F	0.43	0/1801	0.67	1/2444 (0.0%)
All	All	0.47	2/10607 (0.0%)	0.81	46/14391 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	94	PRO	N-CD	-14.68	1.27	1.47
1	C	224	PRO	N-CD	5.50	1.55	1.47

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	114	LEU	CB-CA-C	-15.87	80.06	110.20
1	E	94	PRO	N-CA-CB	-15.17	85.09	103.30
1	C	120	ALA	N-CA-CB	-12.10	93.17	110.10
1	E	94	PRO	CA-N-CD	10.10	125.83	111.70
1	E	93	GLU	CB-CA-C	-10.03	90.35	110.40
1	E	172	GLU	CB-CA-C	-9.80	90.80	110.40
1	E	120	ALA	CB-CA-C	-9.26	96.20	110.10
1	C	109	GLU	N-CA-CB	9.24	127.23	110.60
1	D	103	ILE	CB-CA-C	-8.05	95.51	111.60
1	D	115	GLY	N-CA-C	7.98	133.05	113.10
1	D	172	GLU	CB-CA-C	-7.83	94.75	110.40
1	E	120	ALA	N-CA-C	7.82	132.11	111.00
1	E	172	GLU	N-CA-C	7.61	131.56	111.00
1	D	195	GLU	CB-CA-C	-7.37	95.65	110.40
1	D	109	GLU	N-CA-CB	-7.29	97.48	110.60
1	D	55	ALA	CB-CA-C	-7.10	99.45	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	ASN	N-CA-CB	-7.08	97.86	110.60
1	E	94	PRO	N-CD-CG	-6.94	92.79	103.20
1	D	195	GLU	N-CA-C	6.71	129.13	111.00
1	C	120	ALA	CB-CA-C	-6.60	100.21	110.10
1	C	119	PRO	N-CA-C	6.45	128.86	112.10
1	C	206	VAL	N-CA-CB	-6.43	97.34	111.50
1	C	109	GLU	N-CA-C	-6.28	94.05	111.00
1	B	131	ALA	CB-CA-C	-6.27	100.69	110.10
1	C	206	VAL	N-CA-C	6.22	127.79	111.00
1	D	114	LEU	N-CA-C	6.20	127.73	111.00
1	C	108	ARG	N-CA-C	-6.15	94.39	111.00
1	D	104	ASP	N-CA-CB	-6.15	99.53	110.60
1	D	142	LYS	N-CA-CB	6.11	121.60	110.60
1	D	25	PHE	CB-CA-C	-6.06	98.28	110.40
1	D	117	LEU	CB-CA-C	5.96	121.52	110.20
1	E	94	PRO	N-CA-C	5.82	127.24	112.10
1	D	43	PHE	CB-CA-C	-5.68	99.04	110.40
1	D	120	ALA	CB-CA-C	-5.55	101.78	110.10
1	C	205	GLY	N-CA-C	-5.48	99.41	113.10
1	E	72	SER	N-CA-C	5.47	125.77	111.00
1	F	109	GLU	CB-CA-C	-5.46	99.48	110.40
1	E	97	LYS	CB-CA-C	-5.40	99.60	110.40
1	D	120	ALA	N-CA-C	5.40	125.57	111.00
1	B	109	GLU	CB-CA-C	-5.32	99.76	110.40
1	D	109	GLU	N-CA-C	5.28	125.26	111.00
1	C	131	ALA	CB-CA-C	-5.27	102.19	110.10
1	D	172	GLU	N-CA-C	5.15	124.91	111.00
1	E	96	GLU	CB-CA-C	-5.09	100.21	110.40
1	D	107	ASN	CB-CA-C	5.09	120.57	110.40
1	D	38	SER	N-CA-CB	-5.01	102.99	110.50

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	1747	0	1778	33	0
1	B	1747	0	1778	33	0
1	C	1692	0	1716	41	0
1	D	1670	0	1705	80	0
1	E	1747	0	1778	75	0
1	F	1758	0	1789	47	0
2	A	23	0	0	0	0
2	B	31	0	0	0	0
2	C	18	0	0	1	0
2	D	10	0	0	0	0
2	E	20	0	0	0	0
2	F	22	0	0	1	0
All	All	10485	0	10544	287	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 14.

All (287) 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:89:TYR:CD2	1:D:89:TYR:O	1.90	1.25
1:E:80:LEU:HG	1:E:96:GLU:OE2	1.64	0.97
1:E:80:LEU:O	1:E:96:GLU:HG2	1.72	0.89
1:A:50:GLU:HG2	1:B:179:VAL:HG13	1.52	0.88
1:D:105:ASP:O	1:D:107:ASN:O	1.92	0.87
1:C:204:LYS:HG3	1:C:205:GLY:O	1.76	0.84
1:F:47:CYS:SG	1:F:132:ARG:NH2	2.53	0.82
1:D:18:THR:OG1	1:D:19:THR:N	2.13	0.80
1:A:7:LEU:HD13	1:B:148:LEU:HD13	1.63	0.80
1:B:69:ILE:HG13	1:B:101:PRO:HG2	1.63	0.79
1:D:89:TYR:HD2	1:D:89:TYR:O	1.61	0.75
1:E:87:ASN:O	1:E:92:GLU:O	2.05	0.75
1:A:7:LEU:HB3	1:B:119:PRO:HD3	1.70	0.72
1:C:207:PHE:HB2	1:C:220:TYR:HB2	1.71	0.72
1:D:89:TYR:CG	1:D:89:TYR:O	2.43	0.72
1:E:91:CYS:O	1:E:93:GLU:OE1	2.09	0.70
1:E:172:GLU:OE2	1:E:172:GLU:O	2.09	0.69
1:E:80:LEU:HG	1:E:96:GLU:CD	2.13	0.68
1:B:208:THR:HB	1:B:219:ARG:HG2	1.75	0.68
1:C:197:GLU:HG2	1:C:201:LEU:HB2	1.78	0.65
1:E:5:LEU:HD12	1:E:114:LEU:HD22	1.78	0.65
1:E:93:GLU:OE1	1:E:93:GLU:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:HIS:HB2	1:D:47:CYS:SG	2.37	0.64
1:E:93:GLU:HB2	1:E:94:PRO:HB3	1.78	0.64
1:F:36:LEU:HD23	1:F:69:ILE:HG23	1.80	0.64
1:F:182:LYS:NZ	1:F:185:ASP:OD2	2.27	0.63
1:B:73:ILE:HG21	1:B:108:ARG:CZ	2.27	0.63
1:E:80:LEU:CG	1:E:96:GLU:OE2	2.44	0.63
1:C:121:GLU:O	1:C:129:VAL:HG22	1.99	0.62
1:E:95:THR:OG1	1:E:96:GLU:N	2.30	0.62
1:C:219:ARG:N	2:C:301:HOH:O	2.33	0.61
1:D:16:ALA:H	1:D:23:ILE:HD11	1.65	0.61
1:E:115:GLY:HA3	1:F:6:LEU:HD11	1.82	0.61
1:C:179:VAL:HG13	1:D:50:GLU:HG2	1.82	0.61
1:D:163:VAL:O	1:D:167:LEU:HG	2.00	0.61
1:A:56:LYS:HE2	1:A:90:ASN:HB2	1.83	0.61
1:E:11:ALA:O	1:E:26:HIS:NE2	2.31	0.61
1:D:46:VAL:HB	1:D:132:ARG:HH22	1.65	0.61
1:D:89:TYR:O	1:D:90:ASN:O	2.19	0.61
1:E:150:PRO:HG3	1:F:167:LEU:HD21	1.83	0.61
1:D:13:ASN:HB2	1:D:26:HIS:CE1	2.36	0.60
1:E:167:LEU:HD21	1:F:150:PRO:HG3	1.83	0.60
1:A:148:LEU:HD22	1:B:7:LEU:HG	1.84	0.60
1:D:61:PHE:HB3	1:D:66:VAL:HB	1.84	0.60
1:C:173:LYS:HG3	1:C:224:PRO:HB2	1.83	0.60
1:A:32:SER:HB3	1:A:65:ASN:OD1	2.02	0.59
1:B:36:LEU:HD23	1:B:69:ILE:HG23	1.84	0.59
1:E:33:TRP:CZ3	1:E:144:LYS:HG3	2.37	0.59
1:E:33:TRP:HZ3	1:E:144:LYS:HG3	1.68	0.59
1:A:41:ARG:O	1:A:44:THR:OG1	2.19	0.58
1:E:5:LEU:HD22	1:E:143:LEU:HD22	1.85	0.58
1:D:130:THR:OG1	1:D:131:ALA:N	2.36	0.58
1:B:196:GLU:HA	1:B:199:LYS:HD2	1.86	0.58
1:B:63:LYS:HG3	1:B:64:ARG:HG3	1.85	0.58
1:D:58:ALA:N	1:D:59:PRO:HD2	2.18	0.58
1:E:79:HIS:HB3	1:E:102:ILE:HD12	1.85	0.58
1:E:69:ILE:HG13	1:E:101:PRO:HG2	1.85	0.57
1:D:57:LEU:HD22	1:D:60:GLU:HG3	1.86	0.57
1:E:41:ARG:NH2	1:E:74:ASP:OD1	2.30	0.57
1:B:38:SER:OG	1:B:133:VAL:HG12	2.04	0.57
1:B:38:SER:OG	1:B:131:ALA:O	2.23	0.56
1:D:205:GLY:O	1:D:221:THR:OG1	2.21	0.56
1:D:162:ARG:HD2	1:D:181:TRP:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ASP:HB2	1:D:131:ALA:HB2	1.87	0.56
1:E:24:ARG:HB2	1:E:27:ASP:HB2	1.87	0.56
1:D:72:SER:HB3	1:D:79:HIS:NE2	2.20	0.56
1:B:209:LYS:HB3	1:B:218:LEU:HD23	1.87	0.55
1:F:193:ILE:O	1:F:219:ARG:NH2	2.39	0.55
1:B:50:GLU:OE1	1:B:132:ARG:NH1	2.40	0.55
1:D:39:HIS:CD2	1:D:72:SER:HB2	2.42	0.55
1:B:32:SER:HB3	1:B:65:ASN:OD1	2.06	0.55
1:C:73:ILE:HG12	1:C:129:VAL:HG12	1.88	0.55
1:D:160:ILE:O	1:D:164:VAL:HG23	2.07	0.55
1:A:193:ILE:HD11	1:A:198:ALA:HA	1.89	0.55
1:A:35:ILE:HB	1:A:68:LEU:HD12	1.89	0.55
1:C:108:ARG:O	1:C:112:ILE:HD12	2.05	0.55
1:D:57:LEU:O	1:D:61:PHE:CD2	2.60	0.55
1:E:93:GLU:HG2	1:E:93:GLU:O	2.05	0.55
1:E:136:VAL:HG23	1:E:144:LYS:HB2	1.89	0.54
1:E:179:VAL:HG13	1:F:50:GLU:HG3	1.89	0.54
1:C:90:ASN:O	1:C:92:GLU:HG3	2.08	0.54
1:E:54:ALA:HB2	1:E:157:PHE:CE1	2.44	0.53
1:E:134:VAL:HB	1:E:147:ILE:HG12	1.90	0.53
1:F:41:ARG:NH2	1:F:124:GLU:OE1	2.39	0.53
1:D:25:PHE:O	1:D:25:PHE:CG	2.61	0.53
1:D:177:THR:HB	1:D:181:TRP:CG	2.43	0.53
1:D:164:VAL:HA	1:D:167:LEU:HD11	1.89	0.53
1:F:56:LYS:NZ	1:F:90:ASN:HB2	2.23	0.53
1:D:178:PRO:HD2	1:D:181:TRP:HB2	1.92	0.52
1:D:105:ASP:C	1:D:107:ASN:O	2.48	0.52
1:B:33:TRP:HB2	1:B:66:VAL:HG22	1.90	0.51
1:C:179:VAL:O	1:C:180:ASP:C	2.48	0.51
1:D:132:ARG:C	1:D:155:ARG:HH12	2.13	0.51
1:D:84:LYS:HZ1	1:D:97:LYS:N	2.07	0.51
1:F:35:ILE:HB	1:F:68:LEU:HD12	1.92	0.51
1:C:175:VAL:HG11	1:C:224:PRO:HG2	1.92	0.51
1:C:179:VAL:HG11	1:D:50:GLU:HA	1.92	0.51
1:E:189:VAL:HG22	1:E:202:PHE:CE2	2.46	0.51
1:E:70:ALA:HB2	1:E:100:PHE:HE1	1.76	0.51
1:C:208:THR:HG22	1:C:209:LYS:H	1.75	0.50
1:A:46:VAL:HG13	1:B:178:PRO:HA	1.92	0.50
1:E:178:PRO:HD2	1:E:181:TRP:HB2	1.94	0.50
1:A:173:LYS:HD3	1:A:224:PRO:HB2	1.94	0.50
1:E:142:LYS:HB2	1:E:142:LYS:NZ	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:SER:O	1:E:78:ASP:HB2	2.12	0.50
1:E:40:PRO:HG2	1:E:47:CYS:SG	2.52	0.50
1:F:11:ALA:O	1:F:26:HIS:NE2	2.29	0.50
1:C:118:ASP:HB2	1:C:131:ALA:HB2	1.94	0.50
1:A:211:LEU:O	1:A:214:GLY:N	2.31	0.49
1:E:45:PRO:HD2	1:F:191:PRO:HG3	1.94	0.49
1:B:196:GLU:O	1:B:200:LYS:HG2	2.11	0.49
1:C:208:THR:HG23	1:C:219:ARG:HG3	1.94	0.49
1:D:39:HIS:NE2	1:D:72:SER:HB2	2.27	0.49
1:A:33:TRP:HB2	1:A:66:VAL:HG22	1.94	0.49
1:E:31:ASP:H	1:E:141:LYS:HZ1	1.60	0.49
1:C:162:ARG:HD2	1:C:181:TRP:O	2.12	0.49
1:C:138:GLY:HA3	1:C:144:LYS:HE3	1.94	0.49
1:E:41:ARG:HB3	1:E:44:THR:OG1	2.13	0.49
1:F:132:ARG:NH1	1:F:151:ALA:O	2.41	0.49
1:F:27:ASP:HB3	2:F:308:HOH:O	2.13	0.49
1:E:161:LEU:O	1:E:165:ILE:HG12	2.13	0.49
1:E:32:SER:OG	1:E:65:ASN:OD1	2.21	0.49
1:D:123:ASP:OD2	1:D:123:ASP:N	2.46	0.49
1:F:107:ASN:N	1:F:107:ASN:OD1	2.46	0.49
1:A:50:GLU:OE1	1:A:132:ARG:NH1	2.42	0.48
1:B:45:PRO:O	1:B:49:THR:HG23	2.14	0.48
1:E:70:ALA:O	1:E:103:ILE:N	2.40	0.48
1:B:70:ALA:HB3	1:B:102:ILE:HG12	1.96	0.48
1:E:93:GLU:HB2	1:E:94:PRO:CB	2.42	0.48
1:F:83:SER:HB2	1:F:96:GLU:HA	1.95	0.48
1:C:45:PRO:HD2	1:D:191:PRO:HG3	1.95	0.48
1:D:14:PHE:CZ	1:D:25:PHE:HB2	2.49	0.48
1:D:134:VAL:HB	1:D:147:ILE:HB	1.95	0.48
1:E:60:GLU:HB3	1:E:161:LEU:HD11	1.96	0.48
1:D:141:LYS:O	1:D:141:LYS:HG2	2.13	0.47
1:F:72:SER:HB3	1:F:79:HIS:CE1	2.49	0.47
1:E:40:PRO:HA	1:E:130:THR:HG23	1.97	0.47
1:F:56:LYS:HZ2	1:F:90:ASN:HB2	1.80	0.47
1:A:15:GLU:HA	1:A:23:ILE:O	2.14	0.47
1:A:119:PRO:HD3	1:B:7:LEU:HB3	1.97	0.47
1:C:179:VAL:HB	1:C:180:ASP:OD1	2.15	0.47
1:E:182:LYS:HB2	1:E:182:LYS:HE3	1.72	0.47
1:E:107:ASN:HB2	1:E:109:GLU:HG3	1.97	0.46
1:D:16:ALA:H	1:D:23:ILE:CD1	2.27	0.46
1:E:122:LYS:HA	1:E:128:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:SER:HB3	1:B:98:LEU:HD13	1.97	0.46
1:E:179:VAL:CG1	1:F:50:GLU:HA	2.45	0.46
1:D:44:THR:OG1	1:D:47:CYS:SG	2.72	0.46
1:D:33:TRP:HB2	1:D:66:VAL:HG22	1.98	0.46
1:F:13:ASN:OD1	1:F:24:ARG:HG2	2.16	0.46
1:C:93:GLU:HA	1:C:94:PRO:HD3	1.74	0.45
1:E:179:VAL:CG1	1:F:50:GLU:HG3	2.46	0.45
1:C:93:GLU:O	1:C:95:THR:HG23	2.16	0.45
1:F:182:LYS:HB2	1:F:182:LYS:HE2	1.61	0.45
1:F:18:THR:HG22	1:F:103:ILE:HA	1.99	0.45
1:F:41:ARG:HD2	1:F:74:ASP:OD2	2.16	0.45
1:D:121:GLU:O	1:D:129:VAL:HG11	2.16	0.45
1:B:25:PHE:CZ	1:B:29:LEU:HD21	2.52	0.45
1:D:38:SER:OG	1:D:39:HIS:N	2.49	0.45
1:F:72:SER:HB3	1:F:79:HIS:HE1	1.81	0.45
1:C:45:PRO:CD	1:D:191:PRO:HG3	2.46	0.45
1:D:76:VAL:HA	1:D:79:HIS:HB2	1.99	0.45
1:D:50:GLU:OE2	1:D:132:ARG:NE	2.47	0.45
1:B:82:TRP:O	1:B:86:ILE:HG12	2.16	0.45
1:D:108:ARG:HG2	1:D:128:PRO:HG2	1.98	0.45
1:D:17:ASN:HB2	1:D:106:ARG:NH2	2.32	0.45
1:D:27:ASP:HA	1:D:30:GLY:HA2	1.99	0.45
1:E:68:LEU:O	1:E:100:PHE:HB2	2.16	0.45
1:F:41:ARG:HH22	1:F:124:GLU:CD	2.19	0.45
1:E:98:LEU:HA	1:E:99:PRO:HD3	1.78	0.44
1:E:73:ILE:O	1:E:73:ILE:HD13	2.17	0.44
1:F:35:ILE:HD13	1:F:136:VAL:HG12	1.98	0.44
1:C:15:GLU:HB3	1:C:22:ARG:NH2	2.33	0.44
1:C:80:LEU:HD12	1:C:80:LEU:HA	1.83	0.44
1:E:71:LEU:HA	1:E:103:ILE:HB	1.99	0.44
1:E:162:ARG:HD2	1:E:181:TRP:O	2.17	0.44
1:E:119:PRO:HD3	1:F:7:LEU:HB3	1.99	0.44
1:C:69:ILE:HD12	1:C:101:PRO:HG2	1.99	0.44
1:E:61:PHE:HB3	1:E:66:VAL:HB	1.99	0.44
1:D:211:LEU:HD21	1:D:218:LEU:HB2	1.99	0.44
1:E:108:ARG:NH1	1:E:128:PRO:O	2.50	0.44
1:F:39:HIS:HB2	1:F:47:CYS:SG	2.58	0.44
1:F:111:ALA:HA	1:F:116:MET:HG2	1.99	0.44
1:F:32:SER:HB3	1:F:65:ASN:OD1	2.17	0.44
1:D:22:ARG:HB2	1:D:22:ARG:CZ	2.47	0.44
1:B:147:ILE:HD12	1:B:149:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:LEU:HA	1:D:110:LEU:HD12	1.86	0.44
1:C:200:LYS:HZ3	1:C:201:LEU:N	2.16	0.44
1:F:32:SER:HA	1:F:65:ASN:HD21	1.82	0.44
1:F:136:VAL:HG22	1:F:145:LEU:HB3	1.99	0.43
1:B:138:GLY:HA3	1:B:144:LYS:HE2	2.00	0.43
1:D:71:LEU:HD23	1:D:103:ILE:O	2.18	0.43
1:A:173:LYS:HD3	1:A:224:PRO:CB	2.48	0.43
1:C:75:SER:HA	1:C:106:ARG:HD2	2.01	0.43
1:E:122:LYS:HE2	1:E:128:PRO:HG3	1.99	0.43
1:E:93:GLU:HB2	1:E:94:PRO:CA	2.48	0.43
1:A:204:LYS:HZ2	1:A:204:LYS:H	1.66	0.43
1:B:32:SER:HB3	1:B:65:ASN:CG	2.38	0.43
1:C:124:GLU:OE2	1:C:125:LYS:HE3	2.18	0.43
1:E:72:SER:O	1:E:73:ILE:HG22	2.18	0.43
1:A:104:ASP:OD1	1:A:106:ARG:HD3	2.18	0.43
1:D:132:ARG:HB2	1:D:149:TYR:O	2.18	0.43
1:D:51:LEU:HB2	1:D:86:ILE:HG21	2.00	0.43
1:D:33:TRP:O	1:D:66:VAL:HA	2.18	0.43
1:E:173:LYS:HG2	1:E:224:PRO:HG2	2.00	0.43
1:F:70:ALA:O	1:F:103:ILE:N	2.51	0.43
1:B:147:ILE:HD11	1:B:155:ARG:HG2	2.01	0.43
1:C:104:ASP:OD1	1:C:106:ARG:HD3	2.19	0.43
1:E:33:TRP:CE3	1:E:138:GLY:HA2	2.54	0.43
1:B:201:LEU:HD12	1:B:201:LEU:HA	1.79	0.43
1:A:121:GLU:HG3	1:A:151:ALA:HB3	2.00	0.42
1:C:195:GLU:HA	1:C:198:ALA:HB2	2.01	0.42
1:D:33:TRP:CE3	1:D:138:GLY:HA2	2.53	0.42
1:F:33:TRP:HB2	1:F:66:VAL:HG22	2.00	0.42
1:A:199:LYS:HG3	1:A:199:LYS:H	1.63	0.42
1:A:93:GLU:HA	1:A:94:PRO:HD3	1.83	0.42
1:C:6:LEU:HD23	1:D:117:LEU:HB3	2.00	0.42
1:D:138:GLY:C	1:D:140:ASP:H	2.23	0.42
1:F:118:ASP:OD2	1:F:119:PRO:HD2	2.19	0.42
1:B:194:PRO:HD2	1:B:197:GLU:HB3	2.00	0.42
1:B:15:GLU:HG3	1:B:24:ARG:HD2	2.01	0.42
1:D:87:ASN:HD22	1:D:98:LEU:HD13	1.83	0.42
1:A:15:GLU:HB2	1:A:24:ARG:HD3	2.01	0.42
1:E:50:GLU:OE1	1:E:132:ARG:NH1	2.53	0.42
1:C:93:GLU:H	1:C:93:GLU:HG3	1.53	0.42
1:E:25:PHE:CE2	1:E:29:LEU:HD11	2.54	0.42
1:A:127:MET:HA	1:A:128:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HD21	1:D:150:PRO:HG3	2.02	0.42
1:E:71:LEU:HD12	1:E:103:ILE:HG21	1.99	0.42
1:E:61:PHE:CD2	1:E:68:LEU:HD21	2.55	0.42
1:D:18:THR:HB	1:D:103:ILE:HG23	2.02	0.42
1:D:14:PHE:CE1	1:D:25:PHE:HB2	2.54	0.42
1:F:93:GLU:HA	1:F:94:PRO:HD3	1.81	0.42
1:D:115:GLY:C	1:D:117:LEU:H	2.23	0.42
1:D:35:ILE:HD11	1:D:164:VAL:HG21	2.00	0.42
1:D:58:ALA:N	1:D:59:PRO:CD	2.83	0.42
1:E:118:ASP:OD1	1:E:119:PRO:HD2	2.20	0.42
1:A:121:GLU:HG3	1:A:151:ALA:CB	2.50	0.42
1:C:209:LYS:HD2	1:C:209:LYS:HA	1.89	0.42
1:E:132:ARG:O	1:E:155:ARG:HD3	2.19	0.42
1:F:173:LYS:O	1:F:175:VAL:N	2.53	0.42
1:C:19:THR:HG22	1:C:80:LEU:HD13	2.02	0.41
1:C:59:PRO:O	1:C:63:LYS:HB3	2.19	0.41
1:D:18:THR:HG22	1:D:21:GLY:O	2.19	0.41
1:A:68:LEU:O	1:A:100:PHE:HB2	2.20	0.41
1:A:193:ILE:HA	1:A:194:PRO:HD3	1.72	0.41
1:B:73:ILE:O	1:B:73:ILE:HG22	2.20	0.41
1:D:164:VAL:O	1:D:168:GLN:HB2	2.20	0.41
1:A:195:GLU:O	1:A:199:LYS:HG3	2.20	0.41
1:F:6:LEU:HD12	1:F:6:LEU:HA	1.83	0.41
1:A:121:GLU:HB3	1:A:129:VAL:HG22	2.03	0.41
1:C:156:ASN:O	1:C:159:GLU:HB3	2.20	0.41
1:E:193:ILE:HA	1:E:194:PRO:HD3	1.95	0.41
1:E:57:LEU:O	1:E:60:GLU:N	2.38	0.41
1:A:204:LYS:HB3	1:A:222:PRO:HG2	2.02	0.41
1:B:174:ARG:HB3	1:B:190:LEU:HD12	2.02	0.41
1:E:64:ARG:HB3	1:E:168:GLN:HE22	1.84	0.41
1:F:120:ALA:O	1:F:122:LYS:HG3	2.20	0.41
1:C:179:VAL:CG1	1:D:50:GLU:HA	2.51	0.41
1:E:14:PHE:CD2	1:E:110:LEU:HD21	2.56	0.41
1:D:190:LEU:HD12	1:D:190:LEU:HA	1.95	0.41
1:E:24:ARG:NE	1:E:24:ARG:H	2.19	0.41
1:E:53:ARG:HA	1:E:53:ARG:HD2	1.82	0.41
1:F:215:LYS:HG2	1:F:216:LYS:H	1.85	0.41
1:D:73:ILE:HD11	1:D:130:THR:HG22	2.02	0.41
1:D:73:ILE:O	1:D:106:ARG:HA	2.21	0.41
1:D:174:ARG:C	1:D:190:LEU:HD22	2.40	0.41
1:D:29:LEU:HA	1:D:29:LEU:HD23	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:GLU:O	1:E:64:ARG:HD3	2.21	0.41
1:A:39:HIS:CE1	1:A:72:SER:HB2	2.56	0.40
1:D:193:ILE:H	1:D:193:ILE:HG13	1.69	0.40
1:D:76:VAL:HG22	1:D:80:LEU:HD13	2.02	0.40
1:E:15:GLU:HA	1:E:23:ILE:O	2.22	0.40
1:A:15:GLU:HB2	1:A:24:ARG:NH1	2.36	0.40
1:D:61:PHE:CG	1:D:68:LEU:HD11	2.56	0.40
1:F:56:LYS:HA	1:F:56:LYS:HD2	1.91	0.40
1:A:162:ARG:HD2	1:A:181:TRP:O	2.21	0.40
1:C:63:LYS:HG2	1:C:64:ARG:HG3	2.03	0.40
1:D:190:LEU:HA	1:D:191:PRO:HD3	1.96	0.40
1:E:179:VAL:HG22	1:F:49:THR:OG1	2.22	0.40
1:C:6:LEU:O	1:C:9:ASP:HB2	2.22	0.40
1:D:157:PHE:HA	1:D:160:ILE:HG12	2.03	0.40
1:D:13:ASN:ND2	1:D:26:HIS:H	2.20	0.40
1:F:71:LEU:HA	1:F:103:ILE:HB	2.02	0.40
1:F:39:HIS:CE1	1:F:72:SER:HB2	2.57	0.40
1:F:86:ILE:HD11	1:F:98:LEU:CD1	2.51	0.40
1:D:75:SER:HA	1:D:106:ARG:HG2	2.03	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	219/224 (98%)	201 (92%)	17 (8%)	1 (0%)	29	48
1	B	219/224 (98%)	201 (92%)	18 (8%)	0	100	100
1	C	210/224 (94%)	186 (89%)	23 (11%)	1 (0%)	29	48
1	D	205/224 (92%)	181 (88%)	24 (12%)	0	100	100
1	E	219/224 (98%)	185 (84%)	30 (14%)	4 (2%)	8	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	221/224 (99%)	200 (90%)	20 (9%)	1 (0%)	29	48
All	All	1293/1344 (96%)	1154 (89%)	132 (10%)	7 (0%)	29	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	73	ILE
1	A	19	THR
1	E	25	PHE
1	E	128	PRO
1	C	94	PRO
1	F	73	ILE
1	E	94	PRO

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	192/194 (99%)	177 (92%)	15 (8%)	12	24
1	B	192/194 (99%)	175 (91%)	17 (9%)	9	19
1	C	186/194 (96%)	169 (91%)	17 (9%)	9	18
1	D	183/194 (94%)	149 (81%)	34 (19%)	1	2
1	E	192/194 (99%)	167 (87%)	25 (13%)	4	7
1	F	193/194 (100%)	169 (88%)	24 (12%)	4	9
All	All	1138/1164 (98%)	1006 (88%)	132 (12%)	5	10

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	15	GLU
1	A	17	ASN
1	A	32	SER

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Mol	Chain	Res	Type
1	A	36	LEU
1	A	53	ARG
1	A	68	LEU
1	A	76	VAL
1	A	144	LYS
1	A	161	LEU
1	A	173	LYS
1	A	193	ILE
1	A	204	LYS
1	A	209	LYS
1	A	210	GLU
1	B	24	ARG
1	B	29	LEU
1	B	36	LEU
1	B	76	VAL
1	B	97	LYS
1	B	98	LEU
1	B	113	LEU
1	B	117	LEU
1	B	125	LYS
1	B	140	ASP
1	B	147	ILE
1	B	148	LEU
1	B	158	ASP
1	B	179	VAL
1	B	199	LYS
1	B	201	LEU
1	B	208	THR
1	C	9	ASP
1	C	29	LEU
1	C	36	LEU
1	C	63	LYS
1	C	67	LYS
1	C	76	VAL
1	C	80	LEU
1	C	89	TYR
1	C	119	PRO
1	C	124	GLU
1	C	148	LEU
1	C	161	LEU
1	C	174	ARG
1	C	188	MET

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Mol	Chain	Res	Type
1	C	200	LYS
1	C	210	GLU
1	C	211	LEU
1	D	14	PHE
1	D	23	ILE
1	D	42	ASP
1	D	46	VAL
1	D	49	THR
1	D	51	LEU
1	D	67	LYS
1	D	69	ILE
1	D	73	ILE
1	D	84	LYS
1	D	86	ILE
1	D	89	TYR
1	D	103	ILE
1	D	106	ARG
1	D	107	ASN
1	D	116	MET
1	D	123	ASP
1	D	133	VAL
1	D	140	ASP
1	D	146	SER
1	D	152	THR
1	D	167	LEU
1	D	168	GLN
1	D	172	GLU
1	D	182	LYS
1	D	190	LEU
1	D	192	THR
1	D	196	GLU
1	D	197	GLU
1	D	201	LEU
1	D	206	VAL
1	D	211	LEU
1	D	218	LEU
1	D	221	THR
1	E	5	LEU
1	E	14	PHE
1	E	20	VAL
1	E	24	ARG
1	E	25	PHE

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Mol	Chain	Res	Type
1	E	35	ILE
1	E	36	LEU
1	E	41	ARG
1	E	67	LYS
1	E	73	ILE
1	E	76	VAL
1	E	77	GLU
1	E	80	LEU
1	E	87	ASN
1	E	116	MET
1	E	117	LEU
1	E	118	ASP
1	E	121	GLU
1	E	148	LEU
1	E	161	LEU
1	E	179	VAL
1	E	186	SER
1	E	204	LYS
1	E	216	LYS
1	E	218	LEU
1	F	6	LEU
1	F	14	PHE
1	F	24	ARG
1	F	36	LEU
1	F	56	LYS
1	F	63	LYS
1	F	68	LEU
1	F	69	ILE
1	F	90	ASN
1	F	95	THR
1	F	96	GLU
1	F	97	LYS
1	F	98	LEU
1	F	107	ASN
1	F	124	GLU
1	F	133	VAL
1	F	148	LEU
1	F	161	LEU
1	F	190	LEU
1	F	193	ILE
1	F	201	LEU
1	F	208	THR

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Mol	Chain	Res	Type
1	F	211	LEU
1	F	218	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	221/224 (98%)	-0.25	1 (0%) 91 91	18, 34, 53, 65	0
1	B	221/224 (98%)	-0.24	4 (1%) 68 71	18, 32, 61, 84	0
1	C	214/224 (95%)	0.33	17 (7%) 12 12	17, 36, 114, 126	0
1	D	211/224 (94%)	1.14	53 (25%) 0 0	26, 81, 127, 142	0
1	E	221/224 (98%)	0.47	16 (7%) 15 16	25, 59, 98, 122	0
1	F	223/224 (99%)	-0.09	2 (0%) 84 86	20, 42, 66, 96	0
All	All	1311/1344 (97%)	0.22	93 (7%) 16 16	17, 42, 105, 142	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	ALA	9.0
1	E	97	LYS	8.5
1	D	14	PHE	8.5
1	D	43	PHE	7.6
1	D	113	LEU	7.4
1	D	128	PRO	6.7
1	E	127	MET	6.5
1	D	86	ILE	6.5
1	D	87	ASN	5.9
1	D	112	ILE	5.4
1	D	117	LEU	5.2
1	E	113	LEU	4.8
1	D	80	LEU	4.6
1	D	102	ILE	4.6
1	C	207	PHE	4.4
1	D	108	ARG	4.4
1	C	205	GLY	4.4
1	B	127	MET	4.3
1	D	98	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	17	ASN	4.1
1	D	81	ALA	4.1
1	D	82	TRP	4.0
1	D	126	GLY	4.0
1	C	203	PRO	4.0
1	E	112	ILE	4.0
1	D	25	PHE	4.0
1	C	208	THR	3.9
1	C	206	VAL	3.8
1	D	12	PRO	3.8
1	D	76	VAL	3.7
1	D	78	ASP	3.5
1	E	93	GLU	3.5
1	C	190	LEU	3.5
1	C	194	PRO	3.5
1	D	77	GLU	3.5
1	D	127	MET	3.4
1	C	221	THR	3.3
1	D	125	LYS	3.3
1	D	57	LEU	3.3
1	F	211	LEU	3.3
1	D	103	ILE	3.2
1	D	120	ALA	3.2
1	D	74	ASP	3.2
1	E	120	ALA	3.2
1	A	207	PHE	3.2
1	E	117	LEU	3.2
1	D	73	ILE	3.1
1	F	2	PRO	3.1
1	C	209	LYS	3.0
1	D	56	LYS	3.0
1	E	76	VAL	3.0
1	D	130	THR	2.9
1	D	28	PHE	2.9
1	E	7	LEU	2.9
1	E	203	PRO	2.9
1	C	193	ILE	2.9
1	D	37	PHE	2.9
1	D	84	LYS	2.9
1	D	61	PHE	2.8
1	C	220	TYR	2.8
1	D	68	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	97	LYS	2.7
1	D	109	GLU	2.7
1	D	75	SER	2.7
1	D	124	GLU	2.7
1	C	191	PRO	2.7
1	C	198	ALA	2.6
1	D	89	TYR	2.6
1	D	42	ASP	2.6
1	E	126	GLY	2.6
1	D	27	ASP	2.5
1	D	24	ARG	2.5
1	C	200	LYS	2.4
1	D	69	ILE	2.4
1	D	15	GLU	2.3
1	E	80	LEU	2.3
1	C	184	GLY	2.3
1	D	90	ASN	2.3
1	D	114	LEU	2.3
1	C	192	THR	2.3
1	B	120	ALA	2.3
1	C	210	GLU	2.3
1	E	201	LEU	2.2
1	D	51	LEU	2.2
1	B	125	LYS	2.2
1	E	95	THR	2.2
1	D	71	LEU	2.2
1	B	124	GLU	2.1
1	D	48	THR	2.1
1	E	111	ALA	2.1
1	D	141	LYS	2.1
1	D	199	LYS	2.1
1	E	23	ILE	2.0

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.