



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 02:37 pm GMT

PDB ID : 1A4O
Title : 14-3-3 PROTEIN ZETA ISOFORM
Authors : Liu, D.; Bienkowska, J.; Petosa, C.; Collier, R.J.; Fu, H.; Liddington, R.C.
Deposited on : 1998-02-01
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 ⓘ 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	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

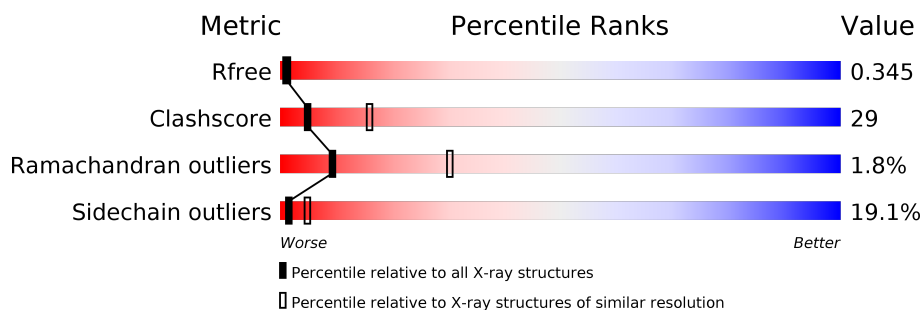
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	245	<div> <div>33%</div> <div>36%</div> <div>11%</div> <div>•</div> <div>20%</div> </div>
1	B	245	<div> <div>31%</div> <div>40%</div> <div>8%</div> <div>•</div> <div>20%</div> </div>
1	C	245	<div> <div>32%</div> <div>38%</div> <div>9%</div> <div>•</div> <div>20%</div> </div>
1	D	245	<div> <div>25%</div> <div>45%</div> <div>10%</div> <div>•</div> <div>20%</div> </div>

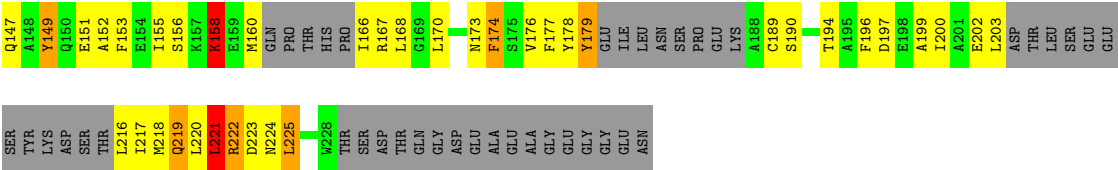
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6360 atoms, of which 0 are hydrogens and 0 are deuteriums.

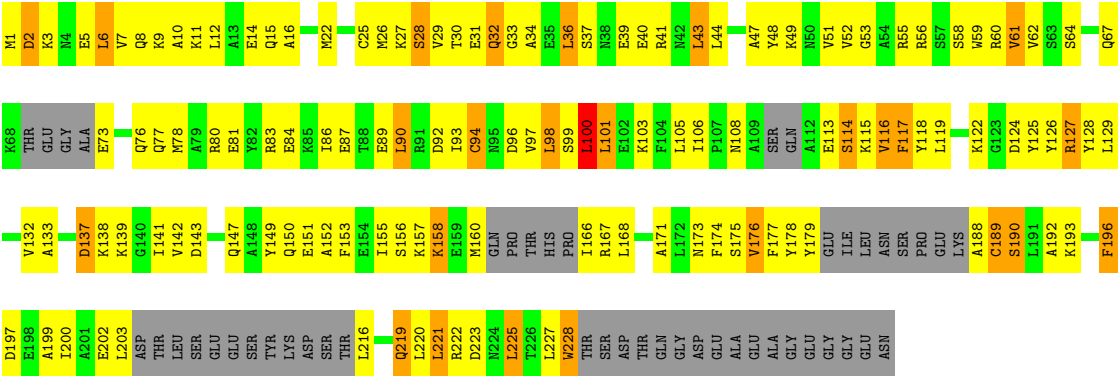
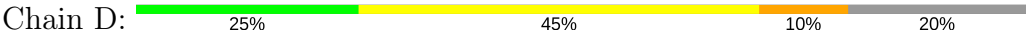
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 14-3-3 PROTEIN ZETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			
1	B	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			
1	C	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			
1	D	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			



● Molecule 1: 14-3-3 PROTEIN ZETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	94.90Å 94.90Å 236.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80 8.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (10.00-2.80) 97.8 (8.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.310 , 0.345 0.317 , 0.345	Depositor DCC
R_{free} test set	2327 reflections (8.21%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.446 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	6360	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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	0.50	1/1605 (0.1%)	0.85	3/2144 (0.1%)
1	B	0.51	0/1605	0.90	6/2144 (0.3%)
1	C	0.49	0/1605	0.85	2/2144 (0.1%)
1	D	0.52	1/1605 (0.1%)	0.89	4/2144 (0.2%)
All	All	0.50	2/6420 (0.0%)	0.87	15/8576 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	CYS	CB-SG	-5.73	1.72	1.81
1	D	94	CYS	CB-SG	-5.12	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	LEU	CA-CB-CG	8.25	134.28	115.30
1	C	221	LEU	CA-CB-CG	7.97	133.63	115.30
1	B	90	LEU	CA-CB-CG	7.16	131.76	115.30
1	B	34	ALA	N-CA-C	6.58	128.76	111.00
1	D	90	LEU	CA-CB-CG	6.37	129.94	115.30
1	A	33	GLY	N-CA-C	-6.20	97.59	113.10
1	B	221	LEU	CA-CB-CG	6.15	129.44	115.30
1	C	90	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	221	LEU	CA-CB-CG	5.99	129.08	115.30
1	B	6	LEU	CA-CB-CG	5.92	128.92	115.30
1	B	33	GLY	N-CA-C	-5.58	99.15	113.10
1	A	90	LEU	CA-CB-CG	5.21	127.29	115.30
1	D	100	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	168	LEU	CA-CB-CG	5.11	127.04	115.30
1	D	33	GLY	N-CA-C	-5.07	100.43	113.10

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	1590	0	1599	86	0
1	B	1590	0	1599	83	0
1	C	1590	0	1599	107	0
1	D	1590	0	1599	108	0
All	All	6360	0	6396	373	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 29.

All (373) 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:30:THR:HG21	1:B:100:LEU:HG	1.56	0.85
1:C:196:PHE:CE1	1:C:200:ILE:HD11	2.13	0.83
1:C:116:VAL:HG11	1:C:160:MET:CE	2.10	0.82
1:B:14:GLU:HB2	1:B:22:MET:SD	2.19	0.81
1:A:216:LEU:HG	1:A:220:LEU:CD1	2.12	0.80
1:A:192:ALA:O	1:A:196:PHE:HB3	1.82	0.80
1:A:67:GLN:OE1	1:A:68:LYS:HG3	1.82	0.79
1:A:113:GLU:HG3	1:A:114:SER:N	1.99	0.77
1:A:216:LEU:HG	1:A:220:LEU:HD11	1.67	0.76
1:D:116:VAL:HG11	1:D:160:MET:SD	2.25	0.76
1:C:219:GLN:NE2	1:C:223:ASP:HB2	2.01	0.75
1:D:58:SER:HB3	1:D:86:ILE:HD13	1.67	0.75
1:D:89:GLU:O	1:D:93:ILE:HG12	1.85	0.75
1:A:27:LYS:HG3	1:A:100:LEU:HD21	1.70	0.73
1:C:153:PHE:HA	1:C:170:LEU:HD21	1.70	0.73
1:C:173:ASN:HA	1:C:176:VAL:HG12	1.71	0.72
1:D:174:PHE:O	1:D:177:PHE:HB3	1.88	0.72
1:C:166:ILE:HG23	1:C:167:ARG:H	1.54	0.72
1:C:178:TYR:O	1:C:179:TYR:HB2	1.90	0.72
1:A:94:CYS:O	1:A:98:LEU:HB2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:VAL:HG23	1:D:29:VAL:HG21	1.71	0.72
1:B:113:GLU:O	1:B:116:VAL:HG12	1.91	0.71
1:C:116:VAL:HG11	1:C:160:MET:HE1	1.73	0.71
1:D:119:LEU:HD23	1:D:151:GLU:HB3	1.71	0.71
1:B:56:ARG:O	1:B:60:ARG:HG3	1.92	0.69
1:A:10:ALA:HB2	1:A:25:CYS:HB2	1.74	0.69
1:A:174:PHE:O	1:A:177:PHE:HB3	1.93	0.68
1:C:200:ILE:HG23	1:C:203:LEU:CD1	2.23	0.68
1:D:156:SER:HA	1:D:160:MET:CE	2.23	0.68
1:B:120:LYS:HG3	1:B:170:LEU:HD12	1.74	0.68
1:D:30:THR:OG1	1:D:105:LEU:HD11	1.93	0.68
1:D:14:GLU:HB2	1:D:22:MET:SD	2.34	0.68
1:A:155:ILE:O	1:A:155:ILE:HG22	1.92	0.68
1:B:109:ALA:CB	1:B:115:LYS:HG2	2.24	0.67
1:A:30:THR:HG21	1:A:100:LEU:HG	1.76	0.67
1:C:168:LEU:HD21	1:C:218:MET:HG2	1.77	0.67
1:C:87:GLU:HG2	1:C:132:VAL:HG13	1.78	0.66
1:D:116:VAL:HG11	1:D:160:MET:HE1	1.77	0.66
1:D:196:PHE:O	1:D:200:ILE:HG13	1.95	0.66
1:B:116:VAL:HG11	1:B:160:MET:CE	2.25	0.66
1:D:97:VAL:HA	1:D:100:LEU:HD22	1.77	0.66
1:B:30:THR:CG2	1:B:100:LEU:HG	2.26	0.65
1:D:116:VAL:HG11	1:D:160:MET:CE	2.27	0.65
1:A:101:LEU:HD12	1:A:105:LEU:HD23	1.78	0.65
1:C:85:LYS:O	1:C:89:GLU:HG3	1.96	0.65
1:B:119:LEU:HB3	1:B:152:ALA:HB2	1.78	0.65
1:C:73:GLU:HA	1:C:76:GLN:HB3	1.79	0.65
1:D:127:ARG:HD3	1:D:149:TYR:OH	1.98	0.64
1:B:200:ILE:HG22	1:B:200:ILE:O	1.98	0.64
1:B:216:LEU:O	1:B:220:LEU:HD13	1.98	0.64
1:B:116:VAL:HG11	1:B:160:MET:HE1	1.79	0.64
1:D:101:LEU:HA	1:D:105:LEU:HB2	1.79	0.64
1:A:106:ILE:HG22	1:A:118:TYR:HB3	1.81	0.63
1:A:221:LEU:O	1:A:225:LEU:HD22	1.98	0.63
1:B:58:SER:O	1:B:62:VAL:HG12	1.99	0.63
1:A:116:VAL:HG23	1:A:152:ALA:HB1	1.80	0.63
1:A:47:ALA:O	1:A:51:VAL:HG23	1.99	0.63
1:C:77:GLN:O	1:C:81:GLU:HB2	1.98	0.63
1:D:49:LYS:HA	1:D:52:VAL:HG12	1.79	0.63
1:D:94:CYS:O	1:D:98:LEU:HB2	1.99	0.62
1:B:3:LYS:HG3	1:B:29:VAL:HG13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:HA	1:C:105:LEU:HB2	1.80	0.62
1:D:77:GLN:O	1:D:81:GLU:HB2	1.99	0.62
1:D:192:ALA:HB3	1:D:225:LEU:HD11	1.80	0.62
1:A:178:TYR:O	1:A:179:TYR:HB2	2.00	0.61
1:A:127:ARG:HD3	1:A:149:TYR:OH	2.00	0.61
1:A:14:GLU:HB2	1:A:22:MET:SD	2.41	0.61
1:A:92:ASP:O	1:A:96:ASP:HB2	2.01	0.61
1:D:92:ASP:O	1:D:96:ASP:HB2	2.00	0.61
1:D:3:LYS:HG3	1:D:29:VAL:HG22	1.82	0.61
1:A:116:VAL:HG11	1:A:160:MET:CE	2.30	0.60
1:C:122:LYS:HE2	1:C:126:TYR:HE2	1.66	0.60
1:C:153:PHE:O	1:C:156:SER:HB2	2.01	0.60
1:C:194:THR:O	1:C:197:ASP:HB3	2.01	0.60
1:D:156:SER:HA	1:D:160:MET:HE2	1.83	0.60
1:A:193:LYS:HA	1:A:196:PHE:HD2	1.67	0.60
1:A:101:LEU:HA	1:A:105:LEU:HB2	1.83	0.60
1:D:124:ASP:O	1:D:127:ARG:HB3	2.02	0.60
1:A:216:LEU:HG	1:A:220:LEU:HD13	1.83	0.59
1:C:92:ASP:O	1:C:96:ASP:HB2	2.02	0.59
1:D:101:LEU:HD12	1:D:105:LEU:HD22	1.85	0.59
1:C:90:LEU:HD21	1:C:132:VAL:HG21	1.83	0.59
1:A:219:GLN:HE21	1:A:223:ASP:HB2	1.67	0.58
1:D:173:ASN:O	1:D:176:VAL:HG12	2.04	0.58
1:B:9:LYS:HD2	1:B:25:CYS:SG	2.44	0.58
1:B:48:TYR:O	1:B:52:VAL:HG12	2.03	0.58
1:C:56:ARG:O	1:C:60:ARG:HG3	2.04	0.58
1:A:27:LYS:O	1:A:30:THR:HG22	2.04	0.58
1:A:176:VAL:HG23	1:A:228:TRP:HZ2	1.68	0.57
1:D:133:ALA:HB2	1:D:141:ILE:HD12	1.86	0.57
1:A:90:LEU:HD21	1:A:132:VAL:HG21	1.85	0.57
1:B:92:ASP:O	1:B:96:ASP:HB2	2.05	0.57
1:A:122:LYS:O	1:A:126:TYR:HD2	1.87	0.57
1:B:7:VAL:HG23	1:B:29:VAL:HG21	1.86	0.57
1:B:109:ALA:HB1	1:B:115:LYS:HG2	1.86	0.57
1:C:106:ILE:HG12	1:C:107:PRO:HD3	1.85	0.57
1:D:58:SER:O	1:D:62:VAL:HG12	2.05	0.56
1:A:99:SER:O	1:A:103:LYS:HB2	2.05	0.56
1:A:73:GLU:O	1:A:76:GLN:HB3	2.05	0.56
1:C:14:GLU:HB2	1:C:22:MET:SD	2.46	0.56
1:D:199:ALA:O	1:D:202:GLU:HB3	2.05	0.56
1:C:75:LYS:O	1:C:78:MET:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PHE:O	1:B:177:PHE:HB3	2.06	0.56
1:D:27:LYS:O	1:D:30:THR:HG22	2.06	0.56
1:C:31:GLU:HA	1:C:104:PHE:CE2	2.41	0.56
1:B:149:TYR:O	1:B:153:PHE:HB2	2.04	0.56
1:B:45:SER:O	1:B:49:LYS:HB3	2.06	0.56
1:A:116:VAL:HG13	1:A:166:ILE:HD11	1.87	0.55
1:A:56:ARG:O	1:A:60:ARG:HG3	2.06	0.55
1:D:178:TYR:O	1:D:179:TYR:HB2	2.05	0.55
1:B:155:ILE:HG22	1:B:155:ILE:O	2.05	0.55
1:C:97:VAL:HA	1:C:100:LEU:HD22	1.88	0.55
1:D:73:GLU:O	1:D:76:GLN:HB3	2.06	0.55
1:B:143:ASP:O	1:B:147:GLN:HG2	2.06	0.55
1:B:39:GLU:O	1:B:43:LEU:HB2	2.07	0.55
1:D:166:ILE:HG23	1:D:167:ARG:H	1.72	0.55
1:B:75:LYS:O	1:B:78:MET:HG3	2.07	0.54
1:D:219:GLN:NE2	1:D:223:ASP:HB2	2.22	0.54
1:C:46:VAL:HA	1:C:49:LYS:HG2	1.89	0.54
1:D:139:LYS:O	1:D:142:VAL:HG12	2.07	0.54
1:C:143:ASP:O	1:C:147:GLN:HG2	2.08	0.54
1:A:30:THR:CG2	1:A:100:LEU:HG	2.38	0.54
1:C:216:LEU:O	1:C:220:LEU:HD13	2.08	0.54
1:C:87:GLU:CG	1:C:132:VAL:HG13	2.37	0.54
1:C:67:GLN:OE1	1:C:68:LYS:HG3	2.07	0.54
1:B:178:TYR:O	1:B:179:TYR:HB2	2.08	0.54
1:B:67:GLN:OE1	1:B:68:LYS:HG3	2.07	0.54
1:C:89:GLU:O	1:C:93:ILE:HG12	2.07	0.54
1:A:48:TYR:O	1:A:52:VAL:HG12	2.08	0.54
1:C:130:ALA:O	1:C:138:LYS:HE3	2.08	0.53
1:D:150:GLN:HA	1:D:153:PHE:HB3	1.89	0.53
1:D:9:LYS:HD2	1:D:25:CYS:SG	2.47	0.53
1:B:119:LEU:HD23	1:B:151:GLU:HB3	1.90	0.53
1:C:36:LEU:HD22	1:C:105:LEU:HD11	1.91	0.53
1:D:6:LEU:HG	1:D:28:SER:HB3	1.89	0.53
1:B:35:GLU:HA	1:B:35:GLU:OE1	2.09	0.53
1:D:133:ALA:HB3	1:D:138:LYS:HA	1.91	0.53
1:D:113:GLU:O	1:D:166:ILE:HD11	2.08	0.53
1:A:9:LYS:HD2	1:A:25:CYS:SG	2.49	0.52
1:A:27:LYS:O	1:A:31:GLU:HG2	2.10	0.52
1:B:52:VAL:HG11	1:B:125:TYR:CE2	2.45	0.52
1:D:171:ALA:O	1:D:175:SER:HB2	2.10	0.52
1:B:73:GLU:O	1:B:76:GLN:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:HA	1:B:100:LEU:HD22	1.92	0.52
1:D:155:ILE:O	1:D:158:LYS:HB3	2.09	0.52
1:C:106:ILE:CG1	1:C:107:PRO:HD3	2.40	0.52
1:B:87:GLU:HG3	1:B:132:VAL:HG22	1.90	0.52
1:D:48:TYR:O	1:D:52:VAL:HG12	2.10	0.52
1:A:93:ILE:O	1:A:97:VAL:HG12	2.09	0.52
1:B:173:ASN:O	1:B:176:VAL:HG12	2.09	0.52
1:C:219:GLN:HE22	1:C:223:ASP:HB2	1.75	0.52
1:D:216:LEU:O	1:D:220:LEU:HD13	2.10	0.52
1:C:200:ILE:HG23	1:C:203:LEU:HD12	1.91	0.51
1:B:189:CYS:HA	1:B:225:LEU:HD11	1.91	0.51
1:A:116:VAL:HG11	1:A:160:MET:HE1	1.91	0.51
1:A:113:GLU:O	1:A:166:ILE:HD11	2.11	0.51
1:A:37:SER:HB3	1:A:40:GLU:HG3	1.93	0.51
1:D:101:LEU:HD12	1:D:105:LEU:CD2	2.40	0.51
1:C:113:GLU:HG3	1:C:114:SER:N	2.25	0.51
1:C:2:ASP:O	1:C:6:LEU:HD22	2.11	0.51
1:D:94:CYS:HB2	1:D:129:LEU:HD13	1.92	0.51
1:D:44:LEU:HD21	1:D:105:LEU:HD21	1.92	0.51
1:D:56:ARG:O	1:D:60:ARG:HG3	2.10	0.51
1:C:200:ILE:HG23	1:C:203:LEU:HD11	1.91	0.50
1:D:27:LYS:O	1:D:31:GLU:HG2	2.11	0.50
1:D:52:VAL:HG11	1:D:125:TYR:HE1	1.75	0.50
1:A:193:LYS:O	1:A:197:ASP:N	2.45	0.50
1:B:116:VAL:HG23	1:B:152:ALA:HB1	1.93	0.50
1:A:129:LEU:HB3	1:A:141:ILE:HG21	1.94	0.50
1:A:156:SER:O	1:A:158:LYS:N	2.43	0.50
1:A:103:LYS:HE3	1:D:31:GLU:O	2.11	0.50
1:B:153:PHE:O	1:B:156:SER:HB2	2.11	0.50
1:C:17:GLU:O	1:C:17:GLU:HG2	2.12	0.50
1:D:133:ALA:CB	1:D:138:LYS:HA	2.41	0.50
1:A:16:ALA:HA	1:B:61:VAL:HG11	1.94	0.50
1:B:222:ARG:O	1:B:225:LEU:HB2	2.11	0.50
1:C:156:SER:O	1:C:158:LYS:N	2.44	0.50
1:B:17:GLU:HG2	1:B:17:GLU:O	2.11	0.49
1:C:222:ARG:HA	1:C:225:LEU:HD22	1.94	0.49
1:D:113:GLU:HG3	1:D:114:SER:N	2.27	0.49
1:A:5:GLU:O	1:A:9:LYS:HB2	2.12	0.49
1:B:121:MET:O	1:B:125:TYR:HD1	1.95	0.49
1:B:22:MET:SD	1:B:47:ALA:HB2	2.53	0.49
1:C:113:GLU:O	1:C:166:ILE:HD11	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LYS:NZ	1:A:158:LYS:HB2	2.26	0.49
1:A:66:GLU:HG3	1:A:76:GLN:HG3	1.93	0.49
1:A:115:LYS:HB3	1:A:115:LYS:NZ	2.28	0.49
1:B:10:ALA:HB2	1:B:25:CYS:HB2	1.94	0.49
1:C:160:MET:HE3	1:C:167:ARG:HB2	1.94	0.49
1:D:106:ILE:HG22	1:D:118:TYR:HB3	1.94	0.49
1:B:103:LYS:HE3	1:C:31:GLU:O	2.12	0.49
1:B:97:VAL:HG11	1:B:125:TYR:CD2	2.48	0.49
1:B:221:LEU:O	1:B:225:LEU:HD22	2.13	0.49
1:D:122:LYS:O	1:D:126:TYR:HD2	1.95	0.49
1:C:117:PHE:CD1	1:C:117:PHE:C	2.86	0.49
1:C:27:LYS:HA	1:C:30:THR:HG22	1.94	0.49
1:A:28:SER:O	1:A:32:GLN:NE2	2.46	0.48
1:D:200:ILE:C	1:D:202:GLU:H	2.16	0.48
1:A:153:PHE:O	1:A:156:SER:HB2	2.13	0.48
1:C:73:GLU:CA	1:C:76:GLN:HB3	2.42	0.48
1:C:22:MET:SD	1:C:47:ALA:HB2	2.54	0.48
1:D:192:ALA:O	1:D:196:PHE:HB3	2.13	0.48
1:B:27:LYS:O	1:B:30:THR:HG22	2.13	0.48
1:D:158:LYS:HB2	1:D:158:LYS:NZ	2.28	0.48
1:D:39:GLU:O	1:D:43:LEU:HB2	2.13	0.48
1:A:115:LYS:HZ2	1:A:115:LYS:HB3	1.79	0.48
1:A:106:ILE:HB	1:A:119:LEU:HD11	1.96	0.48
1:A:117:PHE:HB2	1:A:166:ILE:HD12	1.95	0.48
1:B:1:MET:HB2	1:B:32:GLN:OE1	2.13	0.48
1:C:155:ILE:HG22	1:C:155:ILE:O	2.14	0.48
1:C:219:GLN:HE21	1:C:223:ASP:HB2	1.77	0.48
1:C:38:ASN:HA	1:C:41:ARG:HB3	1.95	0.48
1:B:5:GLU:O	1:B:9:LYS:HB2	2.13	0.48
1:C:119:LEU:HD22	1:C:151:GLU:HB3	1.94	0.48
1:D:6:LEU:HB3	1:D:29:VAL:HG23	1.95	0.48
1:C:196:PHE:HA	1:C:199:ALA:HB3	1.95	0.48
1:D:10:ALA:CB	1:D:26:MET:SD	3.01	0.48
1:D:41:ARG:O	1:D:44:LEU:HB3	2.14	0.47
1:D:87:GLU:HA	1:D:90:LEU:HD23	1.96	0.47
1:B:124:ASP:O	1:B:127:ARG:HB3	2.14	0.47
1:A:124:ASP:O	1:A:127:ARG:HB3	2.15	0.47
1:A:176:VAL:HG23	1:A:228:TRP:CZ2	2.48	0.47
1:C:119:LEU:HB2	1:C:152:ALA:HB2	1.96	0.47
1:D:156:SER:OG	1:D:167:ARG:HG3	2.14	0.47
1:B:85:LYS:O	1:B:89:GLU:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:VAL:HG11	1:C:160:MET:HE2	1.90	0.47
1:D:116:VAL:CG1	1:D:160:MET:HE1	2.42	0.47
1:D:51:VAL:HG13	1:D:55:ARG:NH1	2.29	0.47
1:D:5:GLU:O	1:D:9:LYS:HB2	2.15	0.47
1:D:115:LYS:HB3	1:D:115:LYS:NZ	2.29	0.47
1:D:2:ASP:O	1:D:6:LEU:HD22	2.15	0.47
1:C:124:ASP:O	1:C:127:ARG:HB3	2.15	0.47
1:D:1:MET:HB2	1:D:32:GLN:OE1	2.15	0.47
1:D:7:VAL:CG2	1:D:29:VAL:HG21	2.41	0.47
1:C:6:LEU:HB2	1:C:29:VAL:HG23	1.97	0.47
1:C:1:MET:HB2	1:C:32:GLN:OE1	2.15	0.47
1:A:17:GLU:O	1:A:17:GLU:HG2	2.13	0.47
1:A:97:VAL:HG11	1:A:125:TYR:CD2	2.50	0.47
1:B:127:ARG:O	1:B:131:GLU:HG3	2.15	0.47
1:B:55:ARG:HB3	1:B:90:LEU:HB2	1.95	0.47
1:C:73:GLU:O	1:C:76:GLN:HB3	2.15	0.46
1:C:94:CYS:HB2	1:C:129:LEU:HD13	1.97	0.46
1:D:129:LEU:HB3	1:D:141:ILE:HG21	1.96	0.46
1:C:15:GLN:O	1:D:61:VAL:HG21	2.15	0.46
1:D:193:LYS:O	1:D:197:ASP:N	2.48	0.46
1:C:173:ASN:O	1:C:176:VAL:HG12	2.16	0.46
1:C:119:LEU:CD2	1:C:151:GLU:HB3	2.46	0.46
1:C:106:ILE:HG22	1:C:118:TYR:HB3	1.97	0.46
1:A:115:LYS:O	1:A:119:LEU:HD13	2.15	0.46
1:D:59:TRP:CE2	1:D:83:ARG:HD3	2.50	0.46
1:A:90:LEU:CD2	1:A:132:VAL:HG21	2.46	0.46
1:A:66:GLU:CG	1:A:76:GLN:HG3	2.46	0.46
1:A:98:LEU:HA	1:A:98:LEU:HD12	1.82	0.46
1:D:156:SER:HA	1:D:160:MET:HE3	1.97	0.46
1:D:188:ALA:C	1:D:190:SER:H	2.19	0.46
1:D:94:CYS:CB	1:D:129:LEU:HD13	2.46	0.46
1:A:52:VAL:HG13	1:A:53:GLY:N	2.31	0.45
1:B:171:ALA:O	1:B:175:SER:HB2	2.16	0.45
1:B:86:ILE:O	1:B:90:LEU:HB3	2.16	0.45
1:C:166:ILE:HG23	1:C:167:ARG:N	2.26	0.45
1:D:99:SER:O	1:D:103:LYS:HB2	2.16	0.45
1:B:31:GLU:O	1:C:103:LYS:HE3	2.16	0.45
1:B:34:ALA:HB1	1:B:35:GLU:H	1.44	0.45
1:B:66:GLU:O	1:B:66:GLU:HG2	2.16	0.45
1:C:45:SER:O	1:C:49:LYS:HB3	2.16	0.45
1:D:30:THR:OG1	1:D:36:LEU:HD21	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ARG:O	1:C:131:GLU:HG3	2.16	0.45
1:C:32:GLN:HB3	1:C:33:GLY:H	1.50	0.45
1:C:202:GLU:HG2	1:C:202:GLU:O	2.17	0.45
1:B:155:ILE:O	1:B:155:ILE:CG2	2.64	0.45
1:C:44:LEU:HD21	1:C:105:LEU:HD21	1.99	0.45
1:D:6:LEU:CB	1:D:29:VAL:HG23	2.47	0.45
1:A:216:LEU:O	1:A:220:LEU:HD13	2.17	0.45
1:A:58:SER:O	1:A:62:VAL:HG12	2.17	0.45
1:B:113:GLU:HG3	1:B:114:SER:N	2.32	0.45
1:C:61:VAL:HG11	1:D:16:ALA:HA	1.98	0.45
1:B:160:MET:HB2	1:B:160:MET:HE3	1.94	0.44
1:C:174:PHE:O	1:C:177:PHE:HB3	2.16	0.44
1:B:11:LYS:HG3	1:B:43:LEU:HD21	1.99	0.44
1:D:178:TYR:O	1:D:179:TYR:CB	2.66	0.44
1:A:87:GLU:CG	1:A:132:VAL:HG13	2.47	0.44
1:B:101:LEU:HD12	1:B:105:LEU:HD23	1.98	0.44
1:B:22:MET:HE2	1:B:43:LEU:O	2.17	0.44
1:A:3:LYS:O	1:A:7:VAL:HG23	2.17	0.44
1:C:196:PHE:HE1	1:C:200:ILE:HD11	1.79	0.44
1:D:116:VAL:HG13	1:D:166:ILE:HD11	1.98	0.44
1:C:106:ILE:N	1:C:107:PRO:HD2	2.32	0.44
1:C:196:PHE:CE1	1:C:200:ILE:CD1	2.93	0.44
1:D:133:ALA:CB	1:D:141:ILE:HD12	2.47	0.44
1:B:119:LEU:CB	1:B:152:ALA:HB2	2.45	0.44
1:C:49:LYS:HA	1:C:52:VAL:HG12	1.99	0.44
1:C:94:CYS:O	1:C:98:LEU:HB2	2.17	0.44
1:C:147:GLN:O	1:C:151:GLU:HB2	2.18	0.44
1:C:74:LYS:C	1:C:76:GLN:N	2.71	0.44
1:D:188:ALA:C	1:D:190:SER:N	2.70	0.44
1:A:106:ILE:HB	1:A:119:LEU:CD1	2.48	0.44
1:A:89:GLU:O	1:A:93:ILE:HG12	2.18	0.44
1:D:11:LYS:HG3	1:D:43:LEU:HD21	2.00	0.44
1:D:166:ILE:HG23	1:D:167:ARG:N	2.32	0.44
1:A:2:ASP:O	1:A:6:LEU:HD22	2.18	0.43
1:B:109:ALA:HB3	1:B:115:LYS:HG2	2.00	0.43
1:B:46:VAL:O	1:B:50:ASN:ND2	2.50	0.43
1:C:149:TYR:CE2	1:C:177:PHE:HB2	2.53	0.43
1:B:106:ILE:HG22	1:B:118:TYR:HB3	1.99	0.43
1:C:116:VAL:HG21	1:C:160:MET:HE1	1.99	0.43
1:C:5:GLU:O	1:C:9:LYS:HB2	2.18	0.43
1:D:137:ASP:O	1:D:141:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:HA	1:A:227:LEU:HG	2.00	0.43
1:B:130:ALA:O	1:B:138:LYS:HE3	2.17	0.43
1:C:221:LEU:O	1:C:225:LEU:HD22	2.19	0.43
1:D:189:CYS:HB3	1:D:228:TRP:HE3	1.82	0.43
1:A:77:GLN:O	1:A:81:GLU:HB2	2.18	0.43
1:A:86:ILE:O	1:A:86:ILE:HG22	2.19	0.43
1:A:113:GLU:CG	1:A:114:SER:N	2.77	0.43
1:C:155:ILE:HG23	1:C:158:LYS:HD2	2.01	0.43
1:C:62:VAL:HG23	1:D:12:LEU:HD11	2.00	0.43
1:A:222:ARG:O	1:A:225:LEU:HB2	2.19	0.43
1:A:83:ARG:O	1:A:87:GLU:HB2	2.18	0.43
1:B:18:ARG:H	1:B:18:ARG:HG2	1.63	0.43
1:C:100:LEU:O	1:C:104:PHE:HB2	2.18	0.43
1:C:18:ARG:CZ	1:D:86:ILE:HG12	2.48	0.43
1:D:119:LEU:CB	1:D:152:ALA:HB2	2.48	0.43
1:A:172:LEU:HD13	1:A:221:LEU:HB3	2.01	0.43
1:C:100:LEU:HD13	1:C:100:LEU:N	2.33	0.43
1:C:129:LEU:HA	1:C:129:LEU:HD12	1.84	0.43
1:C:87:GLU:HG2	1:C:132:VAL:CG1	2.47	0.43
1:A:6:LEU:HB3	1:A:29:VAL:HG23	2.01	0.43
1:A:49:LYS:HA	1:A:52:VAL:HG12	2.01	0.42
1:D:37:SER:HB3	1:D:40:GLU:HG3	2.01	0.42
1:D:52:VAL:HG11	1:D:125:TYR:CE1	2.54	0.42
1:D:56:ARG:HD2	1:D:128:TYR:CD2	2.54	0.42
1:B:102:GLU:HA	1:B:106:ILE:HG12	2.00	0.42
1:C:94:CYS:CB	1:C:129:LEU:HD13	2.49	0.42
1:C:217:ILE:HG13	1:C:217:ILE:H	1.51	0.42
1:D:76:GLN:O	1:D:80:ARG:N	2.50	0.42
1:A:62:VAL:HG23	1:B:12:LEU:HD11	2.00	0.42
1:A:133:ALA:CB	1:A:138:LYS:HA	2.50	0.42
1:B:126:TYR:HB3	1:B:145:SER:HB2	2.00	0.42
1:C:117:PHE:HD1	1:C:117:PHE:C	2.22	0.42
1:D:37:SER:O	1:D:40:GLU:N	2.53	0.42
1:C:91:ARG:NH1	1:C:132:VAL:HG12	2.35	0.42
1:C:16:ALA:O	1:C:17:GLU:HB3	2.19	0.42
1:D:117:PHE:C	1:D:117:PHE:CD1	2.92	0.42
1:B:106:ILE:N	1:B:107:PRO:HD2	2.34	0.41
1:C:202:GLU:CG	1:C:202:GLU:O	2.68	0.41
1:C:58:SER:O	1:C:62:VAL:HG12	2.20	0.41
1:D:143:ASP:O	1:D:147:GLN:HG2	2.20	0.41
1:B:103:LYS:HE2	1:B:103:LYS:HB2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLU:HG3	1:B:132:VAL:CG2	2.49	0.41
1:A:57:SER:O	1:A:60:ARG:HB2	2.19	0.41
1:D:81:GLU:HA	1:D:84:GLU:OE1	2.20	0.41
1:B:146:GLN:HB2	1:B:177:PHE:CZ	2.56	0.41
1:C:61:VAL:HG21	1:D:15:GLN:O	2.21	0.41
1:B:200:ILE:CG2	1:B:200:ILE:O	2.68	0.41
1:C:120:LYS:HE2	1:C:120:LYS:HB3	1.79	0.41
1:D:22:MET:HG2	1:D:47:ALA:HB2	2.01	0.41
1:D:52:VAL:HG13	1:D:53:GLY:N	2.36	0.41
1:D:98:LEU:HA	1:D:98:LEU:HD12	1.90	0.41
1:B:217:ILE:H	1:B:217:ILE:HG13	1.60	0.41
1:A:29:VAL:O	1:A:32:GLN:HB2	2.20	0.41
1:C:11:LYS:HG3	1:C:43:LEU:HD21	2.03	0.41
1:D:10:ALA:HB2	1:D:26:MET:SD	2.61	0.41
1:D:200:ILE:HG23	1:D:203:LEU:CD1	2.51	0.41
1:C:153:PHE:CA	1:C:170:LEU:HD21	2.45	0.40
1:A:171:ALA:O	1:A:175:SER:HB2	2.21	0.40
1:A:97:VAL:HA	1:A:100:LEU:HD22	2.03	0.40
1:B:155:ILE:HG12	1:B:158:LYS:HE2	2.02	0.40
1:D:155:ILE:O	1:D:158:LYS:CB	2.69	0.40
1:B:160:MET:CE	1:B:167:ARG:HB2	2.51	0.40
1:B:4:ASN:HA	1:B:7:VAL:HB	2.04	0.40
1:C:173:ASN:CA	1:C:176:VAL:HG12	2.46	0.40
1:C:173:ASN:HA	1:C:176:VAL:CG1	2.47	0.40
1:C:78:MET:HE1	1:D:9:LYS:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	185/245 (76%)	155 (84%)	27 (15%)	3 (2%)	11	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	185/245 (76%)	161 (87%)	20 (11%)	4 (2%)	7	25
1	C	185/245 (76%)	165 (89%)	17 (9%)	3 (2%)	11	34
1	D	185/245 (76%)	158 (85%)	24 (13%)	3 (2%)	11	34
All	All	740/980 (76%)	639 (86%)	88 (12%)	13 (2%)	9	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ALA
1	B	34	ALA
1	B	35	GLU
1	B	101	LEU
1	C	34	ALA
1	C	2	ASP
1	D	34	ALA
1	C	158	LYS
1	A	2	ASP
1	D	158	LYS
1	A	158	LYS
1	B	2	ASP
1	D	2	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/209 (81%)	132 (78%)	37 (22%)	1	3
1	B	169/209 (81%)	138 (82%)	31 (18%)	2	5
1	C	169/209 (81%)	140 (83%)	29 (17%)	2	6
1	D	169/209 (81%)	137 (81%)	32 (19%)	1	5
All	All	676/836 (81%)	547 (81%)	129 (19%)	1	5

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	LEU
1	A	8	GLN
1	A	17	GLU
1	A	18	ARG
1	A	28	SER
1	A	32	GLN
1	A	36	LEU
1	A	43	LEU
1	A	46	VAL
1	A	67	GLN
1	A	78	MET
1	A	81	GLU
1	A	88	THR
1	A	93	ILE
1	A	98	LEU
1	A	100	LEU
1	A	101	LEU
1	A	105	LEU
1	A	108	ASN
1	A	114	SER
1	A	129	LEU
1	A	143	ASP
1	A	158	LYS
1	A	174	PHE
1	A	177	PHE
1	A	179	TYR
1	A	189	CYS
1	A	190	SER
1	A	196	PHE
1	A	197	ASP
1	A	219	GLN
1	A	221	LEU
1	A	222	ARG
1	A	225	LEU
1	A	227	LEU
1	A	228	TRP
1	B	1	MET
1	B	2	ASP
1	B	14	GLU
1	B	17	GLU
1	B	28	SER
1	B	36	LEU

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Mol	Chain	Res	Type
1	B	46	VAL
1	B	49	LYS
1	B	64	SER
1	B	67	GLN
1	B	78	MET
1	B	90	LEU
1	B	96	ASP
1	B	97	VAL
1	B	98	LEU
1	B	100	LEU
1	B	101	LEU
1	B	105	LEU
1	B	108	ASN
1	B	113	GLU
1	B	129	LEU
1	B	132	VAL
1	B	149	TYR
1	B	150	GLN
1	B	189	CYS
1	B	190	SER
1	B	196	PHE
1	B	222	ARG
1	B	225	LEU
1	B	227	LEU
1	B	228	TRP
1	C	1	MET
1	C	6	LEU
1	C	17	GLU
1	C	32	GLN
1	C	36	LEU
1	C	43	LEU
1	C	67	GLN
1	C	81	GLU
1	C	82	TYR
1	C	90	LEU
1	C	96	ASP
1	C	98	LEU
1	C	100	LEU
1	C	101	LEU
1	C	105	LEU
1	C	108	ASN
1	C	114	SER

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Mol	Chain	Res	Type
1	C	117	PHE
1	C	149	TYR
1	C	158	LYS
1	C	174	PHE
1	C	179	TYR
1	C	189	CYS
1	C	190	SER
1	C	219	GLN
1	C	221	LEU
1	C	222	ARG
1	C	224	ASN
1	C	225	LEU
1	D	6	LEU
1	D	8	GLN
1	D	28	SER
1	D	32	GLN
1	D	36	LEU
1	D	43	LEU
1	D	61	VAL
1	D	64	SER
1	D	67	GLN
1	D	78	MET
1	D	98	LEU
1	D	100	LEU
1	D	101	LEU
1	D	108	ASN
1	D	114	SER
1	D	116	VAL
1	D	117	PHE
1	D	127	ARG
1	D	132	VAL
1	D	137	ASP
1	D	157	LYS
1	D	168	LEU
1	D	176	VAL
1	D	189	CYS
1	D	190	SER
1	D	196	PHE
1	D	219	GLN
1	D	221	LEU
1	D	222	ARG
1	D	225	LEU

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Mol	Chain	Res	Type
1	D	227	LEU
1	D	228	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	95	ASN
1	A	146	GLN
1	A	219	GLN
1	B	50	ASN
1	B	95	ASN
1	C	146	GLN
1	C	147	GLN
1	C	150	GLN
1	C	219	GLN
1	D	146	GLN
1	D	219	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.