Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:01 PM GMT

PDB ID	:	1DO5
Title	:	HUMAN COPPER CHAPERONE FOR SUPEROXIDE DISMUTASE DOMAIN II
Authors	:	Lamb, A.L.; Wernimont, A.K.; Pufahl, R.A.; O'Halloran, T.V.; Rosenzweig, A.C.
Deposited on	:	1999-12-18
Resolution	:	2.75 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 (i)) were used in the production of this report:

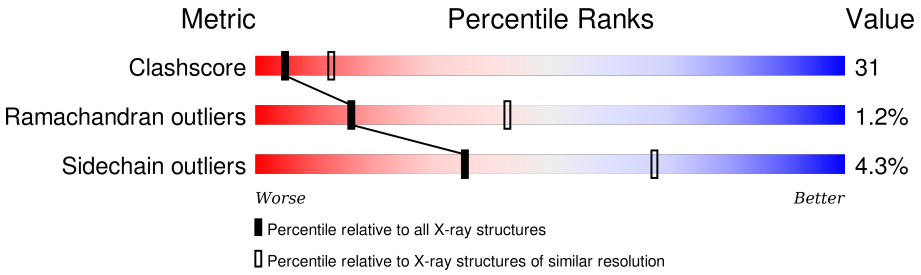
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.75 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))
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	154	53% 45%
1	B	154	45% 47%
1	C	154	46% 48%
1	D	154	51% 43% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4495 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 HUMAN COPPER CHAPERONE FOR SUPEROXIDE DISMUTASE DOMAIN II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1143	696	218	224	5			
1	B	148	Total	C	N	O	S	0	0	0
			1094	664	210	215	5			
1	C	148	Total	C	N	O	S	0	0	0
			1094	664	210	215	5			
1	D	153	Total	C	N	O	S	0	0	0
			1134	691	216	222	5			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	7	Total	O	0	0
			7	7		
3	C	8	Total	O	0	0
			8	8		
3	D	5	Total	O	0	0
			5	5		

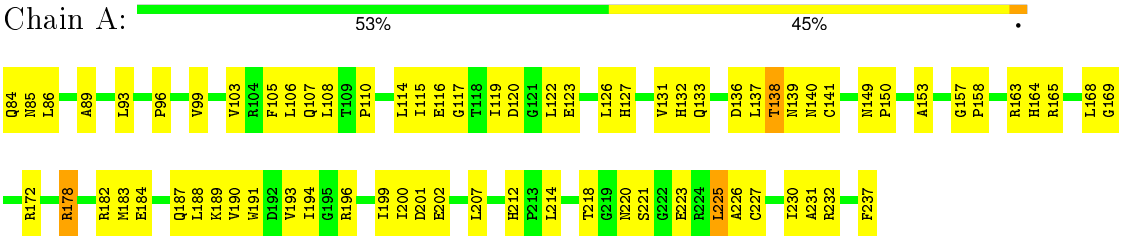
3 Residue-property plots (i)

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.

Note EDS was not executed.

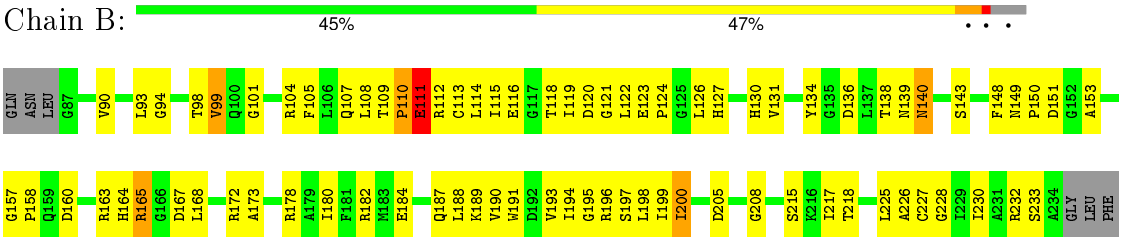
• Molecule 1: HUMAN COPPER CHAPERONE FOR SUPEROXIDE DISMUTASE DOMAIN II

Chain A:



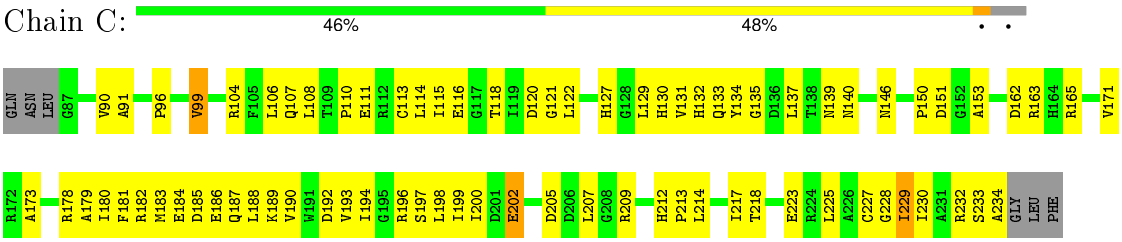
• Molecule 1: HUMAN COPPER CHAPERONE FOR SUPEROXIDE DISMUTASE DOMAIN II

Chain B:



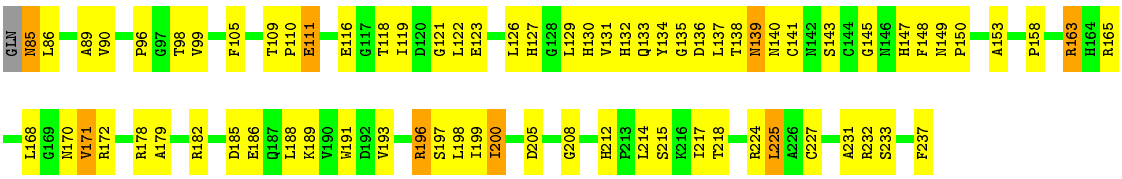
• Molecule 1: HUMAN COPPER CHAPERONE FOR SUPEROXIDE DISMUTASE DOMAIN II

Chain C:



• Molecule 1: HUMAN COPPER CHAPERONE FOR SUPEROXIDE DISMUTASE DOMAIN II

Chain D:


GLN
N85
L86
A89
V90
P96
G97
T98
V99
F105
T109
P110
E111
E116
G117
T118
I119
D120
G121
L122
E123
L126
H127
G128
L129
H130
V131
H132
Q133
Y134
G135
D136
L137
T138
N139
N140
C141
N142
S143
C144
G145
N146
H147
F148
N149
P150
A153
P158
R163
H164
R165
L168
G169
N170
V171
R172
R178
A179
R182
D185
E186
Q187
L188
K189
V190
W191
D192
V193
R196
S197
L198
I199
I200
D205
G208
H212
P213
L214
S215
K216
I217
T218
R224
L225
A226
C227
A231
R232
S233
F237

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.19Å 66.72Å 88.03Å 90.00° 96.63° 90.00°	Depositor
Resolution (Å)	19.21 – 2.75	Depositor
% Data completeness (in resolution range)	90.1 (19.21-2.75)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.228 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4495	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.37	0/1162	0.68	0/1568
1	B	0.35	0/1112	0.66	0/1502
1	C	0.40	0/1112	0.67	0/1502
1	D	0.35	0/1153	0.68	0/1556
All	All	0.37	0/4539	0.67	0/6128

There are no bond length outliers.

There are no bond angle outliers.

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	1143	0	1093	74	0
1	B	1094	0	1045	70	0
1	C	1094	0	1045	84	0
1	D	1134	0	1085	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	0	1	0
3	C	8	0	0	1	0
3	D	5	0	0	1	0
All	All	4495	0	4268	271	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 31.

All (271) 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:150:PRO:HD2	1:B:165:ARG:HG3	1.44	0.94
1:A:212:HIS:HD2	1:A:214:LEU:H	1.17	0.88
1:C:133:GLN:HE21	1:C:146:ASN:H	0.90	0.88
1:D:149:ASN:HD21	1:D:153:ALA:H	1.21	0.87
1:C:90:VAL:HG23	1:C:233:SER:HB2	1.61	0.82
1:D:90:VAL:HG23	1:D:233:SER:HB2	1.59	0.82
1:C:133:GLN:NE2	1:C:146:ASN:H	1.74	0.81
1:D:130:HIS:HE1	1:D:205:ASP:OD2	1.61	0.81
1:B:119:ILE:HG21	1:B:200:ILE:HD13	1.60	0.81
1:B:168:LEU:HD21	1:B:188:LEU:HD22	1.63	0.81
1:B:109:THR:HB	1:B:110:PRO:HD2	1.61	0.80
1:C:133:GLN:HE21	1:C:146:ASN:N	1.75	0.80
1:B:119:ILE:HG21	1:B:200:ILE:CD1	2.12	0.79
1:D:85:ASN:HD22	1:D:85:ASN:N	1.79	0.79
1:A:199:ILE:HG12	1:A:227:CYS:HB3	1.65	0.78
1:D:135:GLY:HA2	1:D:197:SER:HB3	1.66	0.77
1:A:212:HIS:CD2	1:A:214:LEU:H	2.00	0.77
1:A:150:PRO:HD2	1:A:165:ARG:HG3	1.66	0.77
1:D:109:THR:HB	1:D:110:PRO:HD2	1.69	0.74
1:A:99:VAL:HG21	1:A:225:LEU:HD13	1.70	0.73
1:A:149:ASN:HD21	1:A:153:ALA:H	1.38	0.72
1:D:99:VAL:HG11	1:D:200:ILE:HD12	1.71	0.71
1:C:188:LEU:HD11	1:C:193:VAL:HG11	1.73	0.70
1:D:217:ILE:HG22	1:D:218:THR:HG23	1.75	0.68
1:D:89:ALA:HB3	1:D:105:PHE:HB2	1.75	0.68
1:A:199:ILE:HG12	1:A:227:CYS:CB	2.24	0.68
1:D:123:GLU:O	1:D:127:HIS:HE1	1.77	0.68
1:C:212:HIS:CD2	1:C:214:LEU:H	2.12	0.67
1:D:111:GLU:HA	1:D:189:LYS:HE3	1.76	0.67
1:C:202:GLU:HA	1:C:225:LEU:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASP:OD1	1:A:138:THR:HB	1.96	0.66
1:C:212:HIS:HD2	1:C:214:LEU:H	1.44	0.65
1:D:85:ASN:N	1:D:85:ASN:ND2	2.45	0.65
1:B:130:HIS:HE1	1:B:205:ASP:OD2	1.78	0.65
1:C:153:ALA:HB1	1:C:162:ASP:OD1	1.97	0.65
1:B:200:ILE:HG13	1:B:226:ALA:HB3	1.79	0.65
1:C:114:LEU:HD21	1:C:116:GLU:OE2	1.98	0.64
1:C:171:VAL:HG12	1:C:179:ALA:HB1	1.80	0.64
1:C:107:GLN:NE2	1:C:189:LYS:HD2	2.13	0.64
1:C:199:ILE:HG12	1:C:227:CYS:HB3	1.80	0.64
1:D:150:PRO:HG2	1:D:165:ARG:NH1	2.12	0.64
1:D:208:GLY:HA2	1:D:215:SER:O	1.98	0.64
1:B:99:VAL:HG11	1:B:225:LEU:HD13	1.79	0.63
1:A:194:ILE:HD13	1:A:232:ARG:HG2	1.80	0.63
1:A:193:VAL:HA	1:A:196:ARG:HD2	1.80	0.63
1:D:96:PRO:HD2	1:D:225:LEU:O	1.99	0.62
1:C:122:LEU:HD21	1:C:200:ILE:HD13	1.81	0.62
1:A:232:ARG:HD2	1:B:196:ARG:HG2	1.81	0.62
1:B:178:ARG:NE	1:B:180:ILE:HD11	2.15	0.62
1:B:190:VAL:O	1:B:194:ILE:HG23	2.00	0.62
1:D:149:ASN:HD21	1:D:153:ALA:N	1.96	0.62
1:B:178:ARG:CZ	1:B:180:ILE:HD11	2.30	0.62
1:C:115:ILE:HB	1:C:183:MET:HG3	1.82	0.61
1:A:108:LEU:HD12	1:A:184:GLU:OE2	2.00	0.61
1:B:138:THR:HG22	1:C:139:ASN:OD1	2.01	0.61
1:A:123:GLU:O	1:A:127:HIS:HE1	1.83	0.61
1:C:189:LYS:O	1:C:192:ASP:HB2	2.01	0.61
1:D:178:ARG:HD2	3:D:23:HOH:O	2.00	0.60
1:B:157:GLY:H	1:B:160:ASP:HB2	1.65	0.60
1:A:237:PHE:O	1:C:146:ASN:HB3	2.01	0.60
1:D:119:ILE:HG21	1:D:200:ILE:HD13	1.82	0.60
1:A:194:ILE:HG23	1:B:195:GLY:HA3	1.84	0.60
1:C:133:GLN:HG3	1:C:134:TYR:CD1	2.36	0.59
1:B:188:LEU:HD11	1:B:193:VAL:HG11	1.83	0.59
1:C:188:LEU:HD11	1:C:193:VAL:CG1	2.31	0.59
1:A:116:GLU:HG2	1:A:182:ARG:HG3	1.85	0.59
1:A:188:LEU:HD11	1:A:193:VAL:CG1	2.33	0.59
1:B:108:LEU:HD11	1:B:114:LEU:HB2	1.85	0.59
1:A:232:ARG:O	1:B:134:TYR:HB3	2.03	0.58
1:C:122:LEU:HB3	1:C:127:HIS:CE1	2.39	0.58
1:B:139:ASN:O	1:B:140:ASN:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:NH2	1:B:187:GLN:HB3	2.19	0.58
1:C:196:ARG:HG2	1:D:232:ARG:HD2	1.84	0.58
1:B:199:ILE:HG12	1:B:227:CYS:CB	2.34	0.58
1:C:193:VAL:HB	1:C:230:ILE:HD12	1.86	0.57
1:A:149:ASN:HD21	1:A:153:ALA:N	2.00	0.57
1:A:157:GLY:HA2	1:A:207:LEU:HD22	1.85	0.57
1:D:116:GLU:HG2	1:D:182:ARG:HG3	1.86	0.57
1:A:200:ILE:HG23	1:A:225:LEU:HD12	1.85	0.57
1:B:149:ASN:HD21	1:B:153:ALA:H	1.53	0.57
1:B:189:LYS:HG3	1:B:191:TRP:CZ2	2.39	0.57
1:C:115:ILE:HD11	1:C:188:LEU:HD23	1.87	0.57
1:C:228:GLY:O	1:C:229:ILE:HB	2.05	0.57
1:A:133:GLN:O	1:A:196:ARG:NH1	2.37	0.57
1:B:139:ASN:ND2	3:B:13:HOH:O	2.38	0.56
1:D:145:GLY:O	1:D:224:ARG:NH2	2.35	0.56
1:C:99:VAL:HA	1:C:120:ASP:O	2.05	0.56
1:C:217:ILE:HG22	1:C:218:THR:HG23	1.88	0.56
1:A:103:VAL:HG22	1:A:117:GLY:HA3	1.87	0.56
1:A:132:HIS:O	1:A:196:ARG:HB3	2.06	0.56
1:C:135:GLY:HA2	1:C:197:SER:HB3	1.88	0.56
1:B:124:PRO:HA	1:B:173:ALA:O	2.06	0.56
1:D:99:VAL:CG1	1:D:200:ILE:HD12	2.35	0.55
1:B:194:ILE:HD12	1:B:232:ARG:CZ	2.36	0.55
1:C:110:PRO:HG2	1:C:111:GLU:OE2	2.06	0.55
1:A:127:HIS:HD2	1:A:201:ASP:O	1.90	0.55
1:B:107:GLN:OE1	1:B:113:CYS:HB2	2.07	0.55
1:C:130:HIS:HE1	1:C:205:ASP:OD2	1.90	0.54
1:D:136:ASP:OD1	1:D:138:THR:HB	2.07	0.54
1:C:132:HIS:CE1	1:C:199:ILE:HD12	2.42	0.54
1:B:120:ASP:OD1	1:B:178:ARG:HG3	2.08	0.54
1:D:132:HIS:O	1:D:196:ARG:HB3	2.08	0.54
1:C:228:GLY:O	1:C:229:ILE:CB	2.56	0.53
1:B:122:LEU:HD21	1:B:200:ILE:HD12	1.91	0.53
1:A:212:HIS:HD2	1:A:214:LEU:N	1.98	0.53
1:B:90:VAL:HG21	1:B:104:ARG:NH2	2.24	0.53
1:B:99:VAL:HA	1:B:120:ASP:O	2.08	0.53
1:D:212:HIS:HD2	1:D:214:LEU:HB2	1.73	0.53
1:B:151:ASP:OD2	1:B:165:ARG:HD3	2.09	0.53
1:A:132:HIS:CE1	1:A:199:ILE:HD12	2.44	0.53
1:B:199:ILE:HG12	1:B:227:CYS:HB3	1.91	0.53
1:D:119:ILE:HG21	1:D:200:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:HIS:CE1	1:D:199:ILE:HD12	2.44	0.52
1:C:190:VAL:O	1:C:194:ILE:HG23	2.10	0.52
1:B:126:LEU:HD21	1:B:172:ARG:NH1	2.24	0.52
1:C:193:VAL:HG23	1:C:230:ILE:HG21	1.92	0.52
1:B:99:VAL:HG11	1:B:225:LEU:CD1	2.39	0.52
1:A:110:PRO:O	1:A:189:LYS:HE3	2.10	0.52
1:B:139:ASN:CG	1:C:139:ASN:HB2	2.30	0.51
1:D:137:LEU:HA	1:D:140:ASN:O	2.09	0.51
1:A:165:ARG:HD2	1:A:187:GLN:HE21	1.76	0.51
1:D:189:LYS:HD2	1:D:191:TRP:CH2	2.45	0.51
1:A:107:GLN:HB2	1:A:190:VAL:CG2	2.41	0.51
1:A:96:PRO:HD2	1:A:225:LEU:O	2.11	0.51
1:A:188:LEU:HD11	1:A:193:VAL:HG11	1.91	0.51
1:D:199:ILE:HG12	1:D:227:CYS:HB3	1.93	0.51
1:C:114:LEU:HD21	1:C:116:GLU:CD	2.30	0.51
1:C:202:GLU:HB2	1:C:225:LEU:HD21	1.93	0.51
1:D:141:CYS:O	1:D:224:ARG:NH1	2.42	0.50
1:B:101:GLY:HA3	1:B:118:THR:O	2.11	0.50
1:A:193:VAL:HB	1:A:230:ILE:CD1	2.41	0.50
1:C:150:PRO:CG	1:C:165:ARG:HG3	2.40	0.50
1:B:138:THR:CG2	3:C:16:HOH:O	2.59	0.50
1:B:136:ASP:C	1:B:136:ASP:OD1	2.50	0.50
1:B:109:THR:OG1	1:B:112:ARG:HG2	2.12	0.50
1:A:165:ARG:CD	1:A:187:GLN:HE21	2.24	0.50
1:D:99:VAL:HG13	1:D:122:LEU:HG	1.94	0.50
1:C:194:ILE:HD13	1:C:232:ARG:CZ	2.42	0.50
1:A:89:ALA:HA	1:A:231:ALA:O	2.12	0.49
1:C:173:ALA:HA	1:C:179:ALA:HB2	1.93	0.49
1:B:164:HIS:HB2	1:B:167:ASP:CG	2.32	0.49
1:C:116:GLU:OE2	1:C:182:ARG:CZ	2.61	0.49
1:D:193:VAL:HA	1:D:196:ARG:HD2	1.94	0.49
1:C:99:VAL:H	1:C:121:GLY:HA3	1.77	0.49
1:B:123:GLU:O	1:B:127:HIS:HE1	1.95	0.49
1:B:110:PRO:C	1:B:111:GLU:HG3	2.33	0.49
1:A:200:ILE:CG2	1:A:226:ALA:HB3	2.42	0.49
1:D:126:LEU:HD23	1:D:172:ARG:HB2	1.94	0.49
1:D:158:PRO:HG3	1:D:168:LEU:C	2.33	0.49
1:B:188:LEU:CD1	1:B:193:VAL:HG11	2.43	0.48
1:A:158:PRO:HG3	1:A:168:LEU:C	2.34	0.48
1:B:208:GLY:HA2	1:B:215:SER:O	2.13	0.48
1:B:93:LEU:HD23	1:B:228:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ASN:O	1:C:140:ASN:HB2	2.13	0.48
1:A:193:VAL:HG23	1:A:230:ILE:HG21	1.95	0.48
1:A:196:ARG:HG2	1:B:232:ARG:HD2	1.94	0.48
1:A:202:GLU:N	1:A:223:GLU:O	2.45	0.48
1:A:150:PRO:HD2	1:A:165:ARG:CG	2.40	0.48
1:D:147:HIS:HE1	1:D:218:THR:O	1.96	0.48
1:A:106:LEU:O	1:A:114:LEU:N	2.45	0.48
1:C:131:VAL:HA	1:C:197:SER:O	2.14	0.48
1:C:171:VAL:CG1	1:C:179:ALA:HB1	2.42	0.48
1:A:165:ARG:HA	1:A:187:GLN:NE2	2.29	0.47
1:A:108:LEU:HB3	1:C:213:PRO:CB	2.44	0.47
1:C:193:VAL:HA	1:C:196:ARG:HD2	1.95	0.47
1:C:212:HIS:HD2	1:C:214:LEU:HB2	1.80	0.47
1:C:182:ARG:HG2	1:C:182:ARG:HH11	1.80	0.47
1:B:90:VAL:HG21	1:B:104:ARG:HH21	1.80	0.47
1:C:118:THR:OG1	1:C:180:ILE:HG12	2.14	0.47
1:C:163:ARG:HH22	1:C:185:ASP:CG	2.17	0.47
1:A:99:VAL:CG2	1:A:225:LEU:HD13	2.42	0.47
1:D:131:VAL:HG21	1:D:188:LEU:HD21	1.96	0.47
1:A:140:ASN:HA	1:A:140:ASN:HD22	1.56	0.47
1:A:158:PRO:CG	1:A:169:GLY:HA3	2.45	0.47
1:C:137:LEU:HD11	1:C:229:ILE:HG13	1.96	0.46
1:A:158:PRO:HG3	1:A:169:GLY:N	2.30	0.46
1:C:133:GLN:O	1:C:196:ARG:HG2	2.16	0.46
1:A:120:ASP:OD1	1:A:178:ARG:HB2	2.15	0.46
1:D:199:ILE:HG12	1:D:227:CYS:CB	2.46	0.46
1:B:116:GLU:HG2	1:B:182:ARG:HE	1.80	0.46
1:B:218:THR:CG2	1:D:237:PHE:HA	2.46	0.46
1:C:115:ILE:HG22	1:C:181:PHE:HE1	1.81	0.46
1:A:165:ARG:HD2	1:A:187:GLN:HG2	1.98	0.46
1:A:201:ASP:HB3	1:A:221:SER:O	2.15	0.45
1:B:218:THR:HG21	1:D:237:PHE:HA	1.99	0.45
1:C:90:VAL:HG12	1:C:91:ALA:H	1.81	0.45
1:D:89:ALA:HA	1:D:231:ALA:O	2.16	0.45
1:D:86:LEU:N	1:D:86:LEU:HD22	2.32	0.45
1:B:94:GLY:O	1:B:226:ALA:HA	2.16	0.45
1:B:105:PHE:CD2	1:B:115:ILE:HG12	2.51	0.45
1:C:90:VAL:HG21	1:D:136:ASP:OD2	2.15	0.45
1:D:133:GLN:HE21	1:D:145:GLY:HA3	1.82	0.45
1:D:133:GLN:O	1:D:196:ARG:NH1	2.48	0.45
1:B:123:GLU:O	1:B:124:PRO:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:GLU:HA	1:C:225:LEU:CD1	2.43	0.45
1:C:90:VAL:HG12	1:C:91:ALA:N	2.31	0.45
1:D:130:HIS:CE1	1:D:205:ASP:OD2	2.54	0.45
1:A:131:VAL:HG11	1:A:193:VAL:HG12	1.98	0.45
1:D:110:PRO:O	1:D:189:LYS:HE3	2.17	0.45
1:C:150:PRO:HG2	1:C:165:ARG:HG3	1.98	0.45
1:C:107:GLN:NE2	1:C:113:CYS:HB2	2.32	0.45
1:D:129:LEU:HD22	1:D:171:VAL:HG21	1.99	0.45
1:C:129:LEU:HD11	1:C:198:LEU:HD11	1.99	0.44
1:B:217:ILE:HD11	1:D:86:LEU:HD21	1.99	0.44
1:B:131:VAL:HA	1:B:197:SER:O	2.18	0.44
1:D:123:GLU:O	1:D:127:HIS:CE1	2.66	0.44
1:C:113:CYS:O	1:C:184:GLU:HA	2.17	0.44
1:A:93:LEU:HD12	1:A:119:ILE:HD13	1.99	0.44
1:D:163:ARG:HH22	1:D:185:ASP:CG	2.20	0.44
1:C:129:LEU:HD22	1:C:171:VAL:HG21	1.99	0.44
1:B:158:PRO:HG3	1:B:168:LEU:C	2.37	0.44
1:A:105:PHE:CD2	1:A:115:ILE:HG12	2.53	0.43
1:B:198:LEU:O	1:B:227:CYS:HA	2.18	0.43
1:C:118:THR:HG21	1:C:178:ARG:HE	1.84	0.43
1:D:130:HIS:O	1:D:198:LEU:HD12	2.18	0.43
1:A:122:LEU:HD21	1:A:200:ILE:HG12	1.99	0.43
1:C:96:PRO:HD2	1:C:225:LEU:O	2.18	0.43
1:A:172:ARG:HG2	1:A:172:ARG:NH1	2.33	0.43
1:D:118:THR:HA	1:D:179:ALA:O	2.18	0.43
1:C:186:GLU:HG2	1:C:186:GLU:H	1.67	0.43
1:B:148:PHE:CE1	1:B:196:ARG:CZ	3.02	0.43
1:C:122:LEU:HD11	1:C:200:ILE:CD1	2.49	0.43
1:A:172:ARG:HG2	1:A:172:ARG:HH11	1.84	0.43
1:C:234:ALA:HB2	1:D:134:TYR:CZ	2.54	0.43
1:B:148:PHE:CE1	1:B:150:PRO:HG3	2.53	0.43
1:B:164:HIS:HB2	1:B:167:ASP:OD2	2.19	0.43
1:B:139:ASN:HB2	1:C:139:ASN:HB2	2.01	0.43
1:A:189:LYS:HD2	1:A:191:TRP:CZ2	2.54	0.43
1:A:140:ASN:HB3	1:A:141:CYS:H	1.60	0.43
1:D:186:GLU:O	1:D:189:LYS:NZ	2.52	0.42
1:B:113:CYS:O	1:B:184:GLU:HA	2.18	0.42
1:C:209:ARG:HG2	1:C:209:ARG:HH11	1.84	0.42
1:A:200:ILE:HG23	1:A:225:LEU:CD1	2.48	0.42
1:D:98:THR:HG22	1:D:98:THR:O	2.19	0.42
1:D:99:VAL:HG22	1:D:121:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HA	1:A:120:ASP:O	2.19	0.42
1:C:137:LEU:HD22	1:C:227:CYS:SG	2.59	0.42
1:B:163:ARG:HD2	1:B:164:HIS:O	2.20	0.42
1:C:205:ASP:OD1	1:C:207:LEU:N	2.48	0.42
1:D:186:GLU:H	1:D:186:GLU:HG2	1.68	0.42
1:A:108:LEU:HB3	1:C:213:PRO:HB2	2.01	0.42
1:C:205:ASP:OD1	1:C:207:LEU:HD23	2.19	0.42
1:C:90:VAL:CG2	1:C:233:SER:HB2	2.42	0.42
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.84	0.42
1:B:199:ILE:HG12	1:B:227:CYS:HB2	2.01	0.42
1:A:194:ILE:CG2	1:B:195:GLY:HA3	2.48	0.41
1:A:137:LEU:HD22	1:A:227:CYS:SG	2.60	0.41
1:B:98:THR:O	1:B:99:VAL:HB	2.19	0.41
1:A:86:LEU:HD11	1:C:217:ILE:HD12	2.02	0.41
1:D:126:LEU:HD22	1:D:170:ASN:HB3	2.02	0.41
1:B:197:SER:HA	1:B:230:ILE:HG13	2.02	0.41
1:C:207:LEU:O	1:C:209:ARG:HG3	2.20	0.41
1:A:126:LEU:HD23	1:A:172:ARG:HB2	2.03	0.41
1:A:84:GLN:NE2	1:A:85:ASN:H	2.18	0.41
1:C:133:GLN:HG3	1:C:134:TYR:CE1	2.55	0.41
1:A:196:ARG:NH1	1:A:196:ARG:HG2	2.36	0.41
1:D:148:PHE:CZ	1:D:150:PRO:HG3	2.55	0.41
1:C:106:LEU:HG	1:C:108:LEU:HD23	2.02	0.41
1:A:168:LEU:HD21	1:A:188:LEU:HD22	2.02	0.41
1:B:90:VAL:HG23	1:B:233:SER:HB2	2.03	0.41
1:A:107:GLN:HB2	1:A:190:VAL:HG21	2.02	0.41
1:A:163:ARG:CD	1:A:164:HIS:O	2.69	0.41
1:C:131:VAL:HG22	1:C:230:ILE:HD11	2.03	0.40
1:C:135:GLY:O	1:C:229:ILE:HG12	2.21	0.40
1:B:99:VAL:H	1:B:121:GLY:HA3	1.85	0.40
1:C:151:ASP:OD1	1:C:165:ARG:NH1	2.55	0.40
1:A:126:LEU:CD2	1:A:172:ARG:HB2	2.51	0.40
1:C:90:VAL:HG13	1:C:104:ARG:HG2	2.03	0.40
1:D:139:ASN:O	1:D:140:ASN:HB2	2.21	0.40
1:C:114:LEU:HG	1:C:116:GLU:HG3	2.03	0.40
1:A:218:THR:C	1:A:220:ASN:H	2.24	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	152/154 (99%)	141 (93%)	11 (7%)	0	100 100
1	B	146/154 (95%)	126 (86%)	16 (11%)	4 (3%)	6 18
1	C	146/154 (95%)	130 (89%)	14 (10%)	2 (1%)	14 38
1	D	151/154 (98%)	145 (96%)	5 (3%)	1 (1%)	26 59
All	All	595/616 (97%)	542 (91%)	46 (8%)	7 (1%)	16 43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	GLU
1	C	229	ILE
1	D	196	ARG
1	B	99	VAL
1	B	110	PRO
1	B	140	ASN
1	C	99	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	118/118 (100%)	113 (96%)	5 (4%)	36 68
1	B	113/118 (96%)	109 (96%)	4 (4%)	43 75
1	C	113/118 (96%)	110 (97%)	3 (3%)	52 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	117/118 (99%)	109 (93%)	8 (7%)	20 46
All	All	461/472 (98%)	441 (96%)	20 (4%)	35 68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	THR
1	A	139	ASN
1	A	178	ARG
1	A	183	MET
1	A	225	LEU
1	B	111	GLU
1	B	143	SER
1	B	165	ARG
1	B	200	ILE
1	C	187	GLN
1	C	202	GLU
1	C	223	GLU
1	D	85	ASN
1	D	111	GLU
1	D	139	ASN
1	D	143	SER
1	D	163	ARG
1	D	171	VAL
1	D	200	ILE
1	D	225	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	127	HIS
1	A	139	ASN
1	A	140	ASN
1	A	142	ASN
1	A	149	ASN
1	A	187	GLN
1	A	212	HIS
1	B	127	HIS
1	B	130	HIS
1	B	133	GLN

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Mol	Chain	Res	Type
1	B	139	ASN
1	B	140	ASN
1	B	142	ASN
1	B	149	ASN
1	B	164	HIS
1	C	130	HIS
1	C	133	GLN
1	C	140	ASN
1	C	142	ASN
1	C	149	ASN
1	C	212	HIS
1	D	127	HIS
1	D	130	HIS
1	D	133	GLN
1	D	139	ASN
1	D	140	ASN
1	D	142	ASN
1	D	149	ASN
1	D	187	GLN
1	D	212	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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.