Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2023 – 01:49 AM EDT

PDB ID	:	3S5C
Title	:	Crystal Structure of a Hexachlorocyclohexane dehydrochlorinase (LinA) Type2
Authors	:	Kukshal, V.; Macwan, A.S.; Kumar, A.; Ramachandran, R.
Deposited on	:	2011-05-23
Resolution	:	3.50 Å(reported)

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

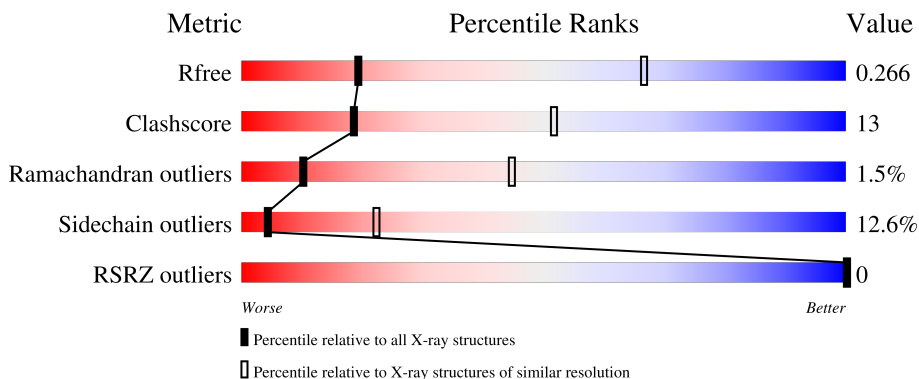|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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	Percentile Ranks	Value
Rfree		0.266
Clashscore		13
Ramachandran outliers		1.5%
Sidechain outliers		12.6%
RSRZ outliers		0

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 of 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 <=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	156	63% 29% ･ ･ ･
1	B	156	65% 26% ･ 5%
1	C	156	67% 24% 6% ･
1	D	156	60% 34% ･ ･ ･
1	E	156	71% 26% ･･

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Mol	Chain	Length	Quality of chain
1	F	156	58% 29% 5% · 6%
1	G	156	62% 27% 7% · ·

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8266 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 LinA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	148	Total	C	N	O	S	0	0	0
			1166	743	198	221	4			
1	A	150	Total	C	N	O	S	0	0	0
			1176	749	200	223	4			
1	C	150	Total	C	N	O	S	0	0	0
			1183	756	202	221	4			
1	D	152	Total	C	N	O	S	0	0	0
			1199	766	204	225	4			
1	E	153	Total	C	N	O	S	0	0	0
			1205	769	205	227	4			
1	F	146	Total	C	N	O	S	0	0	0
			1154	735	196	219	4			
1	G	150	Total	C	N	O	S	0	0	0
			1183	756	202	221	4			

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
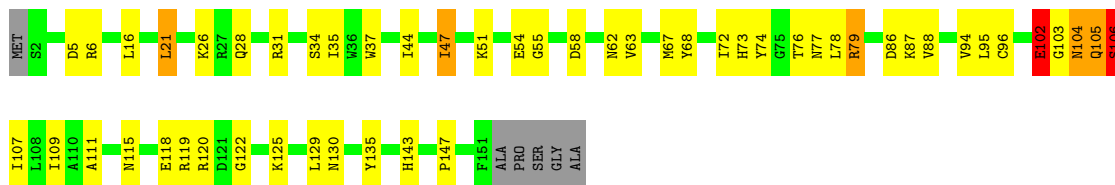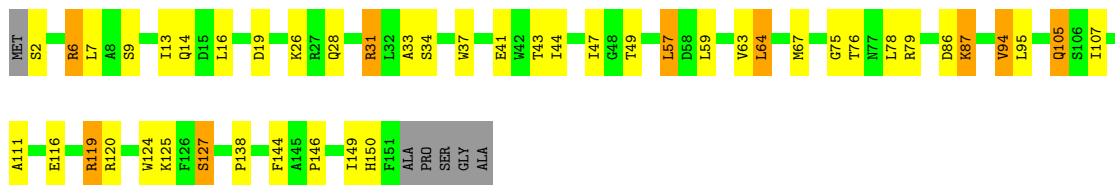
• Molecule 1: LinA

Chain B:
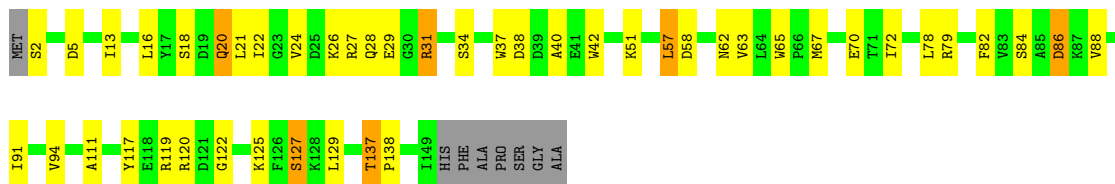
• Molecule 1: LinA

Chain A:

• Molecule 1: LinA

Chain C:

• Molecule 1: LinA

Chain D:

V101 E102 S106 A111 N115 E116 Y117 E118 R119 R120 D121 G122 V123 W124 K125 F126 S127 K128 L129 N130 G131 C132 Y135 A140 F144 A152 P153 SER GLY ALA
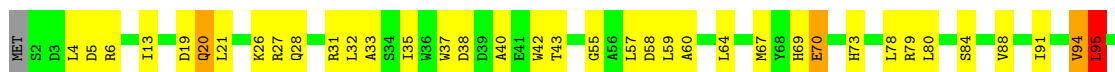
• Molecule 1: LinA

Chain E:

71%　　　　26%　　・・

MET S2 D5 A8 A11 A12 I13 L21 K26 E29 A33 I44 P53 L57 D58 L59 L64 E70 T71 I72 L78 E81 D86 K87 V88 I91 V94 L95 L100 V101 E102 G103 N104 V112 Y113 T114 N115 E116 Y117 E118 R119

V123 W124 L129 N130 M134 I149 H150 F151 A152 P153 S154 GLY ALA
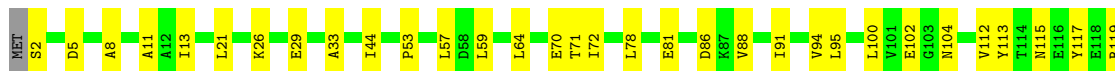
• Molecule 1: LinA

Chain F:

58%　　　　29%　　5% ・ 6%

MET S2 R6 I13 L16 Y17 Q20 L21 K26 E29 I35 W36 W37 W42 T43 T49 Y50 K51 L57 D58 H69 E70 T71 I72 H73 L78 R79 D86 K87 V88 L95 C96 L97 G98 N99 L100 V101 E102 G103 N104 Q105 S106 I107 A110 A111

V112 Y113 T114 Y117 E118 R119 K125 L129 N134 Y135 P138 L139 A140 G141 I142 H143 F144 P147 GLY ILE HIS PHE ALA PRO SER GLY ALA
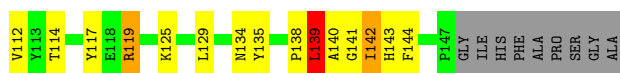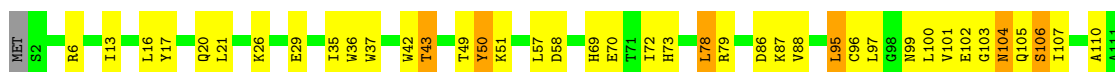
• Molecule 1: LinA

Chain G:

62%　　　　27%　　7% ・・

MET S2 D3 L4 D5 R6 Q14 D19 Q20 L21 V24 R27 Q28 R31 I35 W36 W37 I44 I47 Y50 K51 G52 P53 E54 L57 V63 L64 W65 E70 H73 Y74 N77 L78 R79 F82 K87 V88 N89 G90 I91 G92 D93 V94 L95

S106 I107 E116 Y117 R120 F126 S127 K128 Y135 P138 L139 I142 H143 F144 A145 I149 H150 F151 ALA PRO SER GLY ALA
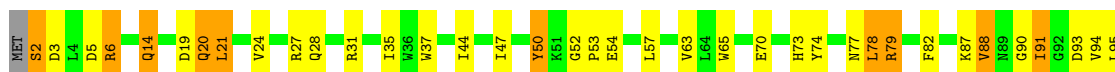
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	162.53Å 162.53Å 186.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.72 – 3.50 30.72 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.72-3.50) 98.8 (30.72-3.50)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.179 , 0.271 0.179 , 0.266	Depositor DCC
R_{free} test set	969 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	58.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 26.3	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8266	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.54	0/1204	0.68	0/1638
1	B	0.55	0/1194	0.71	0/1624
1	C	0.53	0/1213	0.65	0/1650
1	D	0.50	0/1230	0.68	1/1674 (0.1%)
1	E	0.50	0/1236	0.70	0/1682
1	F	0.48	0/1182	0.68	1/1608 (0.1%)
1	G	0.52	0/1213	0.66	0/1650
All	All	0.52	0/8472	0.68	2/11526 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	95	LEU	CA-CB-CG	5.31	127.51	115.30
1	F	95	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1176	0	1127	37	0
1	B	1166	0	1123	28	0
1	C	1183	0	1135	27	0
1	D	1199	0	1151	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1205	0	1156	25	0
1	F	1154	0	1109	40	0
1	G	1183	0	1135	39	0
All	All	8266	0	7936	213	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 13.

All (213) 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:F:42:TRP:CD1	1:F:129:LEU:HD22	2.00	0.94
1:C:107:ILE:HG22	1:C:138:PRO:HA	1.53	0.90
1:F:88:VAL:HG22	1:F:117:TYR:HB2	1.53	0.90
1:B:2:SER:HA	1:B:5:ASP:HB3	1.53	0.90
1:F:104:ASN:O	1:F:143:HIS:HE1	1.58	0.85
1:F:42:TRP:NE1	1:F:129:LEU:HD22	1.92	0.85
1:D:20:GLN:HG3	1:D:21:LEU:N	1.89	0.85
1:D:119:ARG:HD3	1:D:122:GLY:HA2	1.58	0.84
1:E:88:VAL:HG22	1:E:117:TYR:HB2	1.60	0.82
1:D:33:ALA:HB2	1:D:57:LEU:HD21	1.62	0.80
1:D:120:ARG:O	1:D:121:ASP:HB2	1.84	0.76
1:F:86:ASP:OD1	1:F:119:ARG:HD2	1.84	0.76
1:D:28:GLN:NE2	1:D:31:ARG:HE	1.85	0.74
1:F:104:ASN:O	1:F:143:HIS:CE1	2.41	0.73
1:F:138:PRO:O	1:F:139:LEU:HB2	1.87	0.73
1:C:33:ALA:HB2	1:C:57:LEU:HD21	1.69	0.73
1:F:107:ILE:HG22	1:F:138:PRO:HA	1.71	0.71
1:G:79:ARG:O	1:G:90:GLY:HA2	1.91	0.70
1:A:16:LEU:CD2	1:A:35:ILE:HG22	2.23	0.68
1:F:13:ILE:HD13	1:F:88:VAL:HG21	1.74	0.68
1:G:28:GLN:HE22	1:G:31:ARG:HE	1.43	0.65
1:B:28:GLN:NE2	1:B:31:ARG:HE	1.94	0.65
1:D:78:LEU:HD21	1:D:80:LEU:HG	1.77	0.65
1:A:44:ILE:HG22	1:A:47:ILE:HG13	1.78	0.65
1:A:16:LEU:HD23	1:A:35:ILE:HG22	1.78	0.65
1:C:59:LEU:HG	1:C:64:LEU:CD1	2.27	0.64
1:C:94:VAL:HG12	1:C:111:ALA:HB3	1.79	0.64
1:B:88:VAL:CG2	1:B:117:TYR:HB2	2.28	0.64
1:G:107:ILE:HG22	1:G:138:PRO:HA	1.79	0.64
1:G:27:ARG:HA	1:G:65:TRP:CZ2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:LEU:HB2	1:F:105:GLN:HB3	1.81	0.63
1:D:13:ILE:HG21	1:D:80:LEU:HD21	1.81	0.63
1:B:13:ILE:HA	1:B:16:LEU:HD12	1.80	0.62
1:F:112:VAL:HG23	1:F:134:ASN:ND2	2.13	0.62
1:A:86:ASP:OD1	1:A:119:ARG:NH1	2.32	0.61
1:F:99:ASN:ND2	1:G:135:TYR:OH	2.33	0.61
1:B:37:TRP:CH2	1:B:120:ARG:HB2	2.35	0.61
1:B:58:ASP:OD2	1:B:62:ASN:ND2	2.34	0.61
1:D:19:ASP:OD1	1:F:79:ARG:NH1	2.34	0.61
1:B:88:VAL:HG23	1:B:117:TYR:HB2	1.83	0.61
1:B:20:GLN:HG3	1:B:21:LEU:N	2.17	0.60
1:B:34:SER:HB3	1:A:34:SER:HB3	1.84	0.60
1:F:140:ALA:O	1:F:142:ILE:HD12	2.02	0.60
1:E:152:ALA:HB1	1:E:153:PRO:HB3	1.84	0.59
1:A:76:THR:HG21	1:C:76:THR:HG22	1.84	0.59
1:G:52:GLY:C	1:G:54:GLU:H	2.06	0.59
1:A:104:ASN:OD1	1:A:143:HIS:NE2	2.37	0.58
1:D:115:ASN:HD21	1:D:129:LEU:HG	1.68	0.58
1:D:135:TYR:CD1	1:G:144:PHE:HB3	2.38	0.58
1:C:13:ILE:HA	1:C:16:LEU:HD12	1.85	0.57
1:F:17:TYR:CD1	1:F:78:LEU:HG	2.39	0.57
1:A:115:ASN:ND2	1:A:129:LEU:HG	2.18	0.57
1:G:14:GLN:HE21	1:G:78:LEU:HD12	1.69	0.57
1:A:94:VAL:HG12	1:A:111:ALA:HB3	1.87	0.57
1:E:59:LEU:HG	1:E:64:LEU:HD12	1.87	0.57
1:G:88:VAL:HG23	1:G:117:TYR:HB2	1.86	0.57
1:E:112:VAL:HG23	1:E:134:ASN:HD21	1.70	0.57
1:E:149:ILE:HG23	1:E:149:ILE:O	2.05	0.57
1:C:59:LEU:HG	1:C:64:LEU:HD12	1.87	0.56
1:E:100:LEU:O	1:E:104:ASN:HA	2.05	0.56
1:A:37:TRP:CE2	1:A:125:LYS:HB2	2.41	0.56
1:A:68:TYR:HE1	1:A:107:ILE:HD11	1.71	0.56
1:A:119:ARG:HD3	1:A:122:GLY:HA2	1.88	0.56
1:A:96:CYS:HB3	1:A:109:ILE:HB	1.87	0.56
1:F:69:HIS:CD2	1:F:101:VAL:HA	2.40	0.56
1:G:28:GLN:NE2	1:G:31:ARG:HE	2.02	0.56
1:B:27:ARG:HA	1:B:65:TRP:CZ2	2.41	0.56
1:D:33:ALA:HB2	1:D:57:LEU:CD2	2.34	0.56
1:B:37:TRP:CE2	1:B:125:LYS:HB2	2.41	0.56
1:D:117:TYR:CE2	1:D:126:PHE:CE1	2.94	0.56
1:D:37:TRP:CZ2	1:D:120:ARG:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:ASN:HB2	1:G:93:ASP:HB2	1.87	0.55
1:C:107:ILE:HG22	1:C:138:PRO:CA	2.33	0.55
1:B:29:GLU:OE1	1:A:54:GLU:HB2	2.06	0.55
1:E:53:PRO:O	1:E:57:LEU:HD23	2.06	0.55
1:A:94:VAL:CG1	1:A:111:ALA:HB3	2.36	0.55
1:E:44:ILE:HD12	1:E:59:LEU:HD21	1.89	0.55
1:B:119:ARG:HD3	1:B:122:GLY:HA2	1.87	0.55
1:B:94:VAL:HG13	1:B:111:ALA:HB3	1.89	0.55
1:F:106:SER:O	1:F:138:PRO:O	2.26	0.54
1:F:21:LEU:HD22	1:F:73:HIS:HB3	1.90	0.54
1:A:105:GLN:O	1:A:106:SER:HB2	2.08	0.54
1:D:144:PHE:HB3	1:F:135:TYR:CE1	2.42	0.54
1:B:40:ALA:HA	1:B:127:SER:O	2.08	0.53
1:F:144:PHE:HB3	1:G:135:TYR:CD1	2.43	0.53
1:B:20:GLN:HG3	1:B:21:LEU:CD1	2.39	0.53
1:G:116:GLU:HB2	1:G:128:LYS:HB3	1.91	0.53
1:B:84:SER:C	1:B:86:ASP:H	2.12	0.52
1:E:129:LEU:HD12	1:E:130:ASN:N	2.24	0.52
1:A:103:GLY:O	1:A:105:GLN:N	2.41	0.52
1:A:135:TYR:CD1	1:C:144:PHE:HB3	2.45	0.52
1:G:6:ARG:HE	1:G:6:ARG:HA	1.74	0.52
1:C:86:ASP:OD1	1:C:119:ARG:NH1	2.42	0.52
1:C:116:GLU:HB3	1:C:127:SER:HB3	1.91	0.52
1:E:86:ASP:OD1	1:E:119:ARG:NH1	2.38	0.52
1:C:119:ARG:HG3	1:C:124:TRP:CE2	2.45	0.52
1:C:105:GLN:HE21	1:C:105:GLN:HA	1.75	0.51
1:F:29:GLU:HB3	1:F:57:LEU:HD11	1.91	0.51
1:A:87:LYS:HG2	1:A:118:GLU:HG3	1.93	0.51
1:A:63:VAL:O	1:A:67:MET:HB2	2.10	0.51
1:E:2:SER:HA	1:E:5:ASP:HB3	1.92	0.51
1:F:138:PRO:O	1:F:139:LEU:CB	2.57	0.51
1:C:59:LEU:HG	1:C:64:LEU:HD11	1.92	0.51
1:B:28:GLN:HE22	1:B:31:ARG:HE	1.57	0.50
1:B:20:GLN:O	1:B:24:VAL:HG23	2.10	0.50
1:C:37:TRP:CE2	1:C:125:LYS:HB2	2.46	0.50
1:G:20:GLN:O	1:G:24:VAL:HG23	2.12	0.50
1:G:3:ASP:HA	1:G:6:ARG:HB2	1.94	0.50
1:G:149:ILE:O	1:G:149:ILE:HG23	2.12	0.50
1:D:79:ARG:NH1	1:G:19:ASP:OD1	2.44	0.49
1:G:50:TYR:N	1:G:50:TYR:CD1	2.79	0.49
1:A:16:LEU:HD22	1:A:35:ILE:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:GLN:CG	1:D:21:LEU:N	2.69	0.49
1:D:28:GLN:HE22	1:D:31:ARG:HE	1.57	0.49
1:B:82:PHE:HA	1:B:88:VAL:HG12	1.94	0.49
1:B:20:GLN:HG3	1:B:21:LEU:HD12	1.95	0.49
1:C:28:GLN:NE2	1:C:31:ARG:HE	2.11	0.49
1:D:95:LEU:HB2	1:G:74:TYR:CZ	2.47	0.49
1:E:119:ARG:HB2	1:E:124:TRP:CE2	2.48	0.49
1:A:21:LEU:HG	1:A:73:HIS:HB3	1.95	0.48
1:G:21:LEU:HG	1:G:73:HIS:HB3	1.96	0.48
1:E:152:ALA:HB1	1:E:153:PRO:CB	2.44	0.47
1:G:116:GLU:C	1:G:127:SER:HB3	2.34	0.47
1:D:40:ALA:HA	1:D:127:SER:O	2.13	0.47
1:G:145:ALA:HB1	1:G:149:ILE:HG21	1.97	0.47
1:A:44:ILE:CG2	1:A:47:ILE:HG13	2.42	0.47
1:A:105:GLN:HE21	1:A:106:SER:N	2.13	0.47
1:D:31:ARG:HH21	1:F:79:ARG:NH1	2.12	0.47
1:F:50:TYR:N	1:F:50:TYR:CD1	2.83	0.47
1:D:37:TRP:CE2	1:D:125:LYS:HB2	2.50	0.46
1:E:8:ALA:O	1:E:11:ALA:HB3	2.14	0.46
1:A:74:TYR:CZ	1:E:95:LEU:HB2	2.50	0.46
1:F:13:ILE:HA	1:F:16:LEU:HD12	1.97	0.46
1:A:5:ASP:OD1	1:A:119:ARG:NH2	2.48	0.46
1:E:33:ALA:HB2	1:E:57:LEU:HD21	1.98	0.46
1:D:32:LEU:O	1:D:35:ILE:HG12	2.16	0.46
1:E:112:VAL:HG23	1:E:134:ASN:ND2	2.30	0.46
1:A:28:GLN:HE22	1:A:31:ARG:HE	1.64	0.46
1:F:69:HIS:CD2	1:F:101:VAL:HG23	2.50	0.45
1:E:94:VAL:HG11	1:E:113:TYR:CZ	2.51	0.45
1:D:43:THR:HB	1:D:130:ASN:ND2	2.31	0.45
1:D:60:ALA:HA	1:D:64:LEU:HB2	1.98	0.45
1:D:21:LEU:HG	1:D:73:HIS:HB3	1.98	0.45
1:C:7:LEU:HD21	1:E:8:ALA:HA	1.99	0.45
1:C:44:ILE:HB	1:C:47:ILE:HB	1.98	0.45
1:F:43:THR:HG23	1:F:49:THR:OG1	2.17	0.45
1:D:135:TYR:CG	1:G:144:PHE:HB3	2.52	0.45
1:F:110:ALA:HB3	1:F:135:TYR:HB2	1.99	0.45
1:B:137:THR:HA	1:B:138:PRO:HD2	1.87	0.44
1:F:144:PHE:HB3	1:G:135:TYR:CE1	2.52	0.44
1:E:152:ALA:HB1	1:E:153:PRO:CA	2.47	0.44
1:G:2:SER:HA	1:G:5:ASP:HB3	1.99	0.44
1:D:94:VAL:HG12	1:D:111:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:HIS:NE2	1:F:101:VAL:HG23	2.33	0.44
1:C:146:PRO:HD2	1:C:149:ILE:HD12	1.98	0.44
1:E:119:ARG:HA	1:E:123:VAL:O	2.18	0.44
1:G:20:GLN:NE2	1:G:21:LEU:HD12	2.32	0.44
1:G:35:ILE:O	1:G:126:PHE:HB2	2.18	0.44
1:D:13:ILE:HD13	1:D:88:VAL:HG21	2.00	0.44
1:A:79:ARG:NH1	1:C:19:ASP:OD1	2.46	0.43
1:G:20:GLN:HE21	1:G:21:LEU:HD12	1.82	0.43
1:D:115:ASN:ND2	1:D:129:LEU:HG	2.32	0.43
1:E:13:ILE:HD13	1:E:88:VAL:HG21	2.00	0.43
1:G:116:GLU:HB2	1:G:128:LYS:CB	2.47	0.43
1:D:106:SER:HB3	1:D:144:PHE:CD1	2.52	0.43
1:G:44:ILE:O	1:G:47:ILE:HB	2.18	0.43
1:G:50:TYR:OH	1:G:63:VAL:HG21	2.18	0.43
1:A:115:ASN:HD21	1:A:129:LEU:HG	1.82	0.43
1:C:37:TRP:CH2	1:C:120:ARG:HB2	2.53	0.43
1:E:112:VAL:CG2	1:E:134:ASN:HD21	2.31	0.43
1:E:115:ASN:OD1	1:E:129:LEU:HD13	2.18	0.43
1:F:87:LYS:HB2	1:F:87:LYS:HE3	1.77	0.43
1:B:18:SER:O	1:B:22:ILE:HD12	2.18	0.42
1:C:63:VAL:O	1:C:67:MET:HB2	2.18	0.42
1:B:42:TRP:CD1	1:B:129:LEU:HD22	2.55	0.42
1:A:102:GLU:O	1:A:102:GLU:HG3	2.18	0.42
1:F:140:ALA:O	1:F:142:ILE:N	2.52	0.42
1:D:35:ILE:HD12	1:D:126:PHE:CD2	2.54	0.42
1:A:28:GLN:HE21	1:A:28:GLN:HB2	1.64	0.42
1:F:103:GLY:O	1:F:104:ASN:C	2.56	0.42
1:B:84:SER:C	1:B:86:ASP:N	2.73	0.42
1:C:2:SER:O	1:C:6:ARG:NH1	2.52	0.42
1:C:43:THR:OG1	1:C:49:THR:HG23	2.20	0.42
1:F:103:GLY:O	1:F:105:GLN:N	2.53	0.42
1:A:55:GLY:HA2	1:A:58:ASP:HB3	2.01	0.42
1:D:67:MET:O	1:D:101:VAL:HG23	2.20	0.42
1:E:29:GLU:HB3	1:E:57:LEU:HD11	2.00	0.42
1:G:50:TYR:N	1:G:50:TYR:HD1	2.18	0.42
1:G:106:SER:HB3	1:G:144:PHE:CD1	2.55	0.42
1:G:78:LEU:HD23	1:G:78:LEU:HA	1.94	0.42
1:B:63:VAL:HG12	1:B:67:MET:CE	2.50	0.42
1:A:129:LEU:HD23	1:A:130:ASN:N	2.35	0.42
1:C:87:LYS:HE3	1:C:87:LYS:HB2	1.93	0.42
1:B:84:SER:O	1:B:86:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:ARG:HH21	1:F:79:ARG:HH11	1.68	0.41
1:G:79:ARG:HB3	1:G:91:ILE:HG13	2.01	0.41
1:G:106:SER:OG	1:G:143:HIS:HA	2.20	0.41
1:A:28:GLN:HE22	1:A:31:ARG:HH11	1.68	0.41
1:D:55:GLY:HA2	1:D:58:ASP:HB3	2.01	0.41
1:F:112:VAL:HG23	1:F:134:ASN:HD22	1.85	0.41
1:D:42:TRP:CZ3	1:D:59:LEU:HD23	2.56	0.41
1:F:35:ILE:HG13	1:F:36:TRP:CD1	2.55	0.41
1:B:29:GLU:HB3	1:B:57:LEU:HD11	2.01	0.41
1:F:37:TRP:CE2	1:F:125:LYS:HB2	2.56	0.41
1:G:14:GLN:NE2	1:G:78:LEU:HD12	2.35	0.41
1:G:37:TRP:CD2	1:G:120:ARG:HD2	2.55	0.41
1:A:77:ASN:HD21	1:C:75:GLY:H	1.68	0.41
1:D:69:HIS:HB3	1:D:70:GLU:OE2	2.21	0.41
1:F:69:HIS:HD2	1:F:101:VAL:HA	1.86	0.41
1:F:112:VAL:CG2	1:F:134:ASN:ND2	2.82	0.40
1:A:37:TRP:CZ2	1:A:120:ARG:HB2	2.56	0.40
1:A:51:LYS:HB3	1:A:51:LYS:HE2	1.75	0.40
1:C:9:SER:O	1:C:13:ILE:HG13	2.22	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	148/156 (95%)	130 (88%)	14 (10%)	4 (3%)	5	33
1	B	146/156 (94%)	140 (96%)	6 (4%)	0	100	100
1	C	148/156 (95%)	138 (93%)	10 (7%)	0	100	100
1	D	150/156 (96%)	133 (89%)	15 (10%)	2 (1%)	12	48
1	E	151/156 (97%)	140 (93%)	8 (5%)	3 (2%)	7	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	144/156 (92%)	128 (89%)	12 (8%)	4 (3%)	5	32
1	G	148/156 (95%)	132 (89%)	13 (9%)	3 (2%)	7	39
All	All	1035/1092 (95%)	941 (91%)	78 (8%)	16 (2%)	10	45

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	D	140	ALA
1	E	152	ALA
1	F	141	GLY
1	E	102	GLU
1	F	104	ASN
1	G	149	ILE
1	A	102	GLU
1	A	104	ASN
1	F	139	LEU
1	D	152	ALA
1	G	82	PHE
1	F	142	ILE
1	A	147	PRO
1	G	53	PRO
1	E	153	PRO

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	121/126 (96%)	108 (89%)	13 (11%)	6	30
1	B	121/126 (96%)	107 (88%)	14 (12%)	5	26
1	C	122/126 (97%)	105 (86%)	17 (14%)	3	20
1	D	124/126 (98%)	108 (87%)	16 (13%)	4	22
1	E	125/126 (99%)	115 (92%)	10 (8%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	120/126 (95%)	102 (85%)	18 (15%)	3	17
1	G	122/126 (97%)	102 (84%)	20 (16%)	2	13
All	All	855/882 (97%)	747 (87%)	108 (13%)	4	22

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	20	GLN
1	B	26	LYS
1	B	31	ARG
1	B	38	ASP
1	B	51	LYS
1	B	57	LEU
1	B	70	GLU
1	B	72	ILE
1	B	78	LEU
1	B	79	ARG
1	B	86	ASP
1	B	91	ILE
1	B	127	SER
1	B	137	THR
1	A	6	ARG
1	A	21	LEU
1	A	26	LYS
1	A	47	ILE
1	A	62	ASN
1	A	72	ILE
1	A	78	LEU
1	A	79	ARG
1	A	88	VAL
1	A	95	LEU
1	A	102	GLU
1	A	105	GLN
1	A	106	SER
1	C	6	ARG
1	C	14	GLN
1	C	26	LYS
1	C	31	ARG
1	C	34	SER
1	C	41	GLU
1	C	57	LEU

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Mol	Chain	Res	Type
1	C	64	LEU
1	C	78	LEU
1	C	79	ARG
1	C	87	LYS
1	C	94	VAL
1	C	95	LEU
1	C	105	GLN
1	C	119	ARG
1	C	127	SER
1	C	150	HIS
1	D	4	LEU
1	D	5	ASP
1	D	6	ARG
1	D	20	GLN
1	D	26	LYS
1	D	27	ARG
1	D	38	ASP
1	D	70	GLU
1	D	84	SER
1	D	91	ILE
1	D	94	VAL
1	D	95	LEU
1	D	102	GLU
1	D	119	ARG
1	D	123	VAL
1	D	132	CYS
1	E	21	LEU
1	E	26	LYS
1	E	70	GLU
1	E	71	THR
1	E	72	ILE
1	E	78	LEU
1	E	81	GLU
1	E	91	ILE
1	E	150	HIS
1	E	151	PHE
1	F	6	ARG
1	F	20	GLN
1	F	26	LYS
1	F	43	THR
1	F	50	TYR
1	F	51	LYS

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Mol	Chain	Res	Type
1	F	58	ASP
1	F	70	GLU
1	F	72	ILE
1	F	78	LEU
1	F	95	LEU
1	F	96	CYS
1	F	97	LEU
1	F	102	GLU
1	F	106	SER
1	F	114	THR
1	F	119	ARG
1	F	139	LEU
1	G	2	SER
1	G	6	ARG
1	G	14	GLN
1	G	20	GLN
1	G	21	LEU
1	G	50	TYR
1	G	57	LEU
1	G	70	GLU
1	G	78	LEU
1	G	79	ARG
1	G	87	LYS
1	G	88	VAL
1	G	91	ILE
1	G	94	VAL
1	G	95	LEU
1	G	126	PHE
1	G	139	LEU
1	G	142	ILE
1	G	149	ILE
1	G	150	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	28	GLN
1	B	77	ASN
1	A	28	GLN
1	A	77	ASN
1	A	105	GLN
1	A	115	ASN

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Mol	Chain	Res	Type
1	C	28	GLN
1	C	77	ASN
1	C	105	GLN
1	D	28	GLN
1	D	61	ASN
1	D	115	ASN
1	D	130	ASN
1	E	28	GLN
1	E	77	ASN
1	E	134	ASN
1	E	150	HIS
1	F	69	HIS
1	F	99	ASN
1	F	134	ASN
1	F	143	HIS
1	G	14	GLN
1	G	20	GLN
1	G	28	GLN
1	G	77	ASN

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 monosaccharides 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 (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(Å²)	Q<0.9
1	A	150/156 (96%)	-0.72	0	100	100	25, 35, 59, 81	0
1	B	148/156 (94%)	-0.83	0	100	100	20, 30, 39, 53	0
1	C	150/156 (96%)	-0.57	0	100	100	34, 44, 51, 61	0
1	D	152/156 (97%)	-0.58	0	100	100	32, 45, 75, 81	0
1	E	153/156 (98%)	-0.37	0	100	100	30, 52, 67, 85	0
1	F	146/156 (93%)	-0.43	0	100	100	41, 62, 73, 78	0
1	G	150/156 (96%)	-0.14	0	100	100	47, 75, 102, 104	0
All	All	1049/1092 (96%)	-0.52	0	100	100	20, 47, 84, 104	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.