



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:46 pm GMT

PDB ID : 2O74
Title : Structure of OHCU decarboxylase in complex with guanine
Authors : Cendron, L.; Berni, R.; Folli, C.; Ramazzina, I.; Percudani, R.; Zanutti, G.
Deposited on : 2006-12-10
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

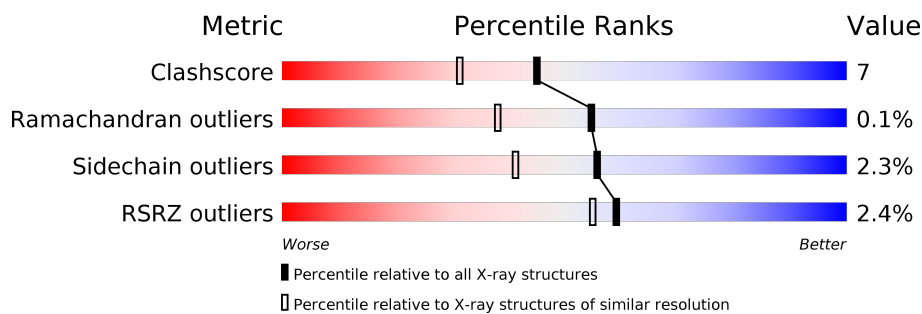
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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 $\leq 5\%$. 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	174	 5% 75% 18% • 5%
1	B	174	 2% 77% 16% • 6%
1	C	174	 2% 84% 11% • •
1	D	174	 2% 81% 12% • 6%
1	E	174	 3% 82% 11% • 6%
1	F	174	 % 87% 9% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GUN	B	2001	-	-	X	-
2	GUN	C	3001	-	-	-	X
2	GUN	F	5001	-	-	-	X

2 Entry composition [i](#)

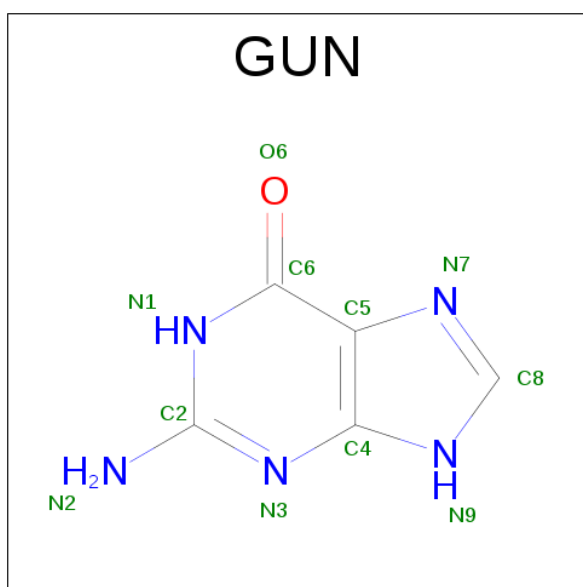
There are 3 unique types of molecules in this entry. The entry contains 8749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OHCU decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1313	826	231	249	7			
1	B	164	Total	C	N	O	S	0	0	0
			1306	821	230	248	7			
1	C	167	Total	C	N	O	S	0	0	0
			1329	837	233	251	8			
1	D	164	Total	C	N	O	S	0	0	0
			1306	821	230	248	7			
1	E	164	Total	C	N	O	S	0	0	0
			1306	821	230	248	7			
1	F	168	Total	C	N	O	S	0	0	0
			1335	840	234	253	8			

- Molecule 2 is GUANINE (three-letter code: GUN) (formula: C₅H₅N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	5	5	1		
2	B	1	Total	C	N	O	0	0
			11	5	5	1		
2	C	1	Total	C	N	O	0	0
			11	5	5	1		
2	D	1	Total	C	N	O	0	0
			11	5	5	1		
2	F	1	Total	C	N	O	0	0
			11	5	5	1		
2	E	1	Total	C	N	O	0	0
			11	5	5	1		

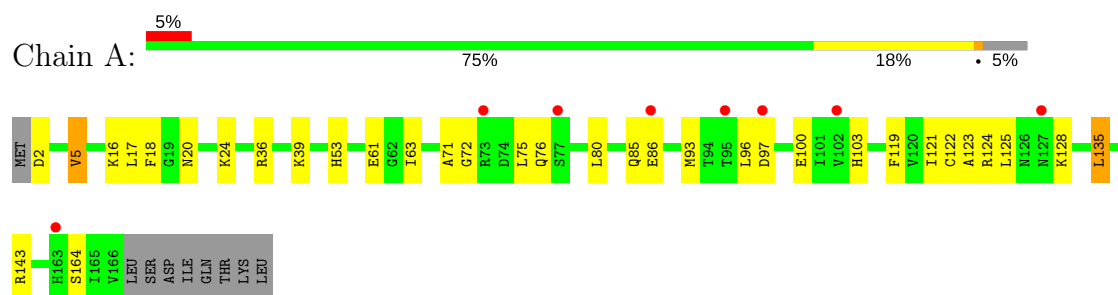
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		
3	B	122	Total	O	0	0
			122	122		
3	C	150	Total	O	0	0
			150	150		
3	D	140	Total	O	0	0
			140	140		
3	E	87	Total	O	0	0
			87	87		
3	F	172	Total	O	0	0
			172	172		

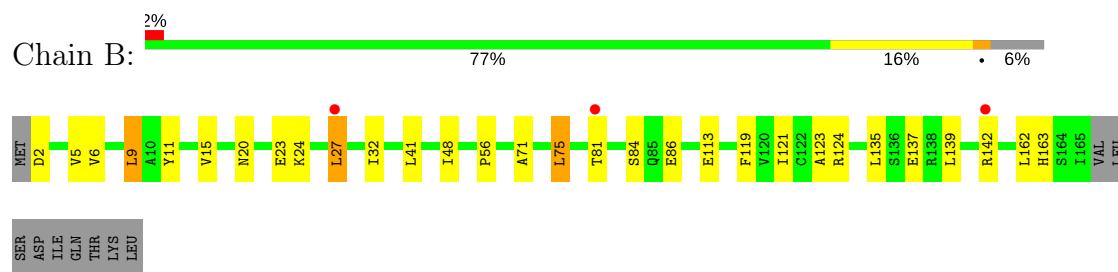
3 Residue-property plots [i](#)

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.

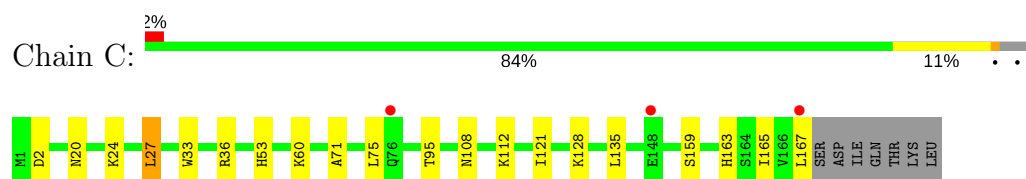
• Molecule 1: OHCU decarboxylase



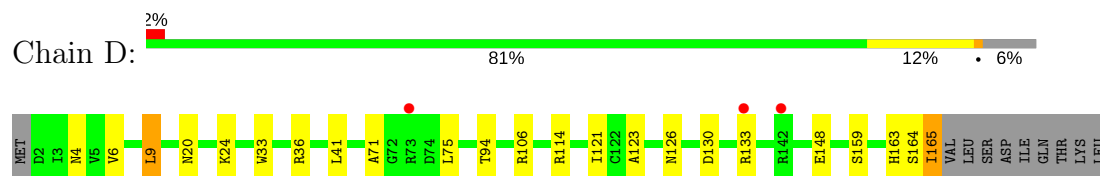
• Molecule 1: OHCU decarboxylase



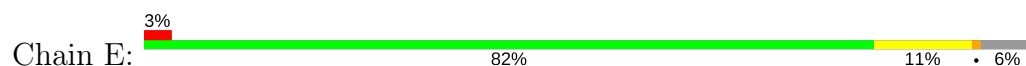
• Molecule 1: OHCU decarboxylase

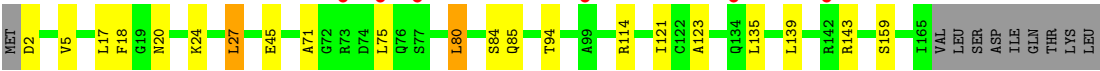


• Molecule 1: OHCU decarboxylase

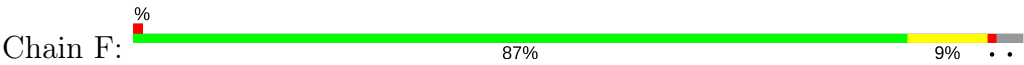


• Molecule 1: OHCU decarboxylase





● Molecule 1: OHCU decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	102.22Å 102.22Å 103.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	88.00 – 1.80 51.11 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (88.00-1.80) 99.6 (51.11-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.257 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l 0.022 for h,-h-k,-l 0.014 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8749	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/1335	0.57	0/1801
1	B	0.45	0/1328	0.60	0/1791
1	C	0.49	0/1351	0.60	1/1822 (0.1%)
1	D	0.48	0/1328	0.56	0/1791
1	E	0.44	0/1328	0.60	1/1791 (0.1%)
1	F	0.49	0/1357	0.58	1/1830 (0.1%)
All	All	0.47	0/8027	0.59	3/10826 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	27	LEU	CA-CB-CG	8.20	134.15	115.30
1	C	27	LEU	CA-CB-CG	7.73	133.07	115.30
1	F	135	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1313	0	1314	33	0
1	B	1306	0	1305	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1329	0	1337	11	0
1	D	1306	0	1305	21	0
1	E	1306	0	1305	13	0
1	F	1335	0	1342	15	0
2	A	11	0	5	3	0
2	B	11	0	5	4	0
2	C	11	0	5	1	0
2	D	11	0	5	2	0
2	E	11	0	5	3	0
2	F	11	0	5	1	0
3	A	117	0	0	9	0
3	B	122	0	0	6	0
3	C	150	0	0	1	0
3	D	140	0	0	5	0
3	E	87	0	0	0	0
3	F	172	0	0	4	0
All	All	8749	0	7938	117	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 7.

All (117) 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:71:ALA:HA	1:D:75:LEU:HD23	1.32	1.06
1:B:27:LEU:HD22	3:B:2122:HOH:O	1.60	1.01
1:A:75:LEU:HA	1:A:80:LEU:HD11	1.02	1.00
1:A:75:LEU:CA	1:A:80:LEU:HD11	1.97	0.94
1:A:75:LEU:HA	1:A:80:LEU:CD1	1.96	0.94
1:A:71:ALA:HA	1:A:75:LEU:HD22	1.48	0.93
1:D:164:SER:O	1:D:165:ILE:HB	1.71	0.89
1:F:71:ALA:HA	1:F:75:LEU:HD23	1.58	0.84
1:E:71:ALA:HA	1:E:75:LEU:HD23	1.65	0.79
1:A:63:ILE:HG13	1:B:27:LEU:HD13	1.64	0.78
1:A:86:GLU:HG3	3:A:1028:HOH:O	1.84	0.76
1:C:95:THR:HG23	3:C:3022:HOH:O	1.88	0.74
1:A:121:ILE:H	2:A:1001:GUN:HN9	1.36	0.74
1:B:6:VAL:HA	1:B:9:LEU:HD22	1.71	0.73
1:A:2:ASP:O	1:A:5:VAL:HG12	1.93	0.69
1:A:20:ASN:HD21	1:A:24:LYS:H	1.42	0.68
1:D:20:ASN:HD21	1:D:24:LYS:H	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ALA:HA	1:A:75:LEU:CD2	2.22	0.67
1:C:20:ASN:ND2	1:C:24:LYS:H	1.93	0.67
1:A:20:ASN:ND2	1:A:24:LYS:H	1.94	0.66
1:F:20:ASN:HD21	1:F:24:LYS:H	1.43	0.66
1:F:119:PHE:CG	1:F:135:LEU:HD13	2.31	0.65
1:C:20:ASN:HD21	1:C:24:LYS:H	1.44	0.65
1:D:24:LYS:HE3	3:D:4034:HOH:O	1.97	0.65
1:A:97:ASP:OD2	3:A:1102:HOH:O	2.14	0.65
1:B:20:ASN:HD21	1:B:24:LYS:H	1.44	0.64
1:C:121:ILE:O	2:C:3001:GUN:N9	2.27	0.64
1:B:124:ARG:HD2	3:B:2011:HOH:O	1.98	0.64
1:B:123:ALA:H	2:B:2001:GUN:HN22	1.47	0.63
1:E:20:ASN:ND2	1:E:24:LYS:H	1.97	0.63
1:C:71:ALA:HA	1:C:75:LEU:HD23	1.79	0.62
1:D:20:ASN:ND2	1:D:24:LYS:H	1.96	0.62
1:E:20:ASN:HD21	1:E:24:LYS:H	1.47	0.61
1:A:124:ARG:NH2	1:A:164:SER:OG	2.34	0.61
1:B:20:ASN:ND2	1:B:24:LYS:H	1.99	0.61
1:F:20:ASN:ND2	1:F:24:LYS:H	2.00	0.60
1:D:123:ALA:H	2:D:4001:GUN:HN22	1.48	0.60
1:D:130:ASP:OD1	1:D:133:ARG:NH2	2.31	0.59
1:A:121:ILE:O	2:A:1001:GUN:N3	2.36	0.59
1:C:53:HIS:HA	1:C:60:LYS:NZ	2.17	0.59
1:F:82:PRO:O	1:F:86:GLU:HG3	2.03	0.58
1:F:119:PHE:CD1	1:F:135:LEU:HD13	2.38	0.58
1:B:23:GLU:OE1	1:B:81:THR:HG21	2.04	0.58
1:A:63:ILE:HG13	1:B:27:LEU:CD1	2.33	0.57
1:B:142:ARG:HG2	3:B:2070:HOH:O	2.05	0.56
1:A:53:HIS:HD2	3:A:1114:HOH:O	1.88	0.56
1:E:75:LEU:HD11	1:E:94:THR:HG22	1.87	0.55
1:B:2:ASP:O	1:B:5:VAL:HG12	2.07	0.54
1:F:95:THR:HG23	3:F:5151:HOH:O	2.07	0.54
1:F:95:THR:CG2	3:F:5136:HOH:O	2.56	0.53
1:F:95:THR:HG21	3:F:5136:HOH:O	2.07	0.53
1:D:148:GLU:HG2	3:D:4137:HOH:O	2.09	0.53
1:E:2:ASP:O	1:E:5:VAL:HG22	2.08	0.53
1:F:121:ILE:O	2:F:5001:GUN:N9	2.27	0.53
1:F:107:LEU:HB3	1:F:135:LEU:HG	1.90	0.52
1:D:121:ILE:O	2:D:4001:GUN:N3	2.43	0.52
1:E:45:GLU:OE2	1:E:159:SER:OG	2.14	0.51
1:B:41:LEU:HD23	1:B:163:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ALA:HA	1:B:75:LEU:HD22	1.93	0.51
1:D:6:VAL:HA	1:D:9:LEU:HD22	1.92	0.51
1:E:121:ILE:O	2:E:6001:GUN:N3	2.43	0.51
1:F:133:ARG:NH1	1:F:134:GLN:OE1	2.44	0.51
1:B:81:THR:HG23	1:B:84:SER:H	1.74	0.51
1:D:71:ALA:HA	1:D:75:LEU:CD2	2.22	0.51
1:E:121:ILE:H	2:E:6001:GUN:HN9	1.58	0.51
1:B:2:ASP:HB3	1:B:5:VAL:HG12	1.92	0.50
1:A:61:GLU:OE2	1:A:143:ARG:NH2	2.44	0.49
1:A:17:LEU:HD23	1:A:18:PHE:CE2	2.48	0.49
1:A:80:LEU:H	1:A:80:LEU:HD12	1.77	0.48
1:F:126:ASN:HD22	1:F:130:ASP:HB3	1.77	0.48
1:C:53:HIS:HA	1:C:60:LYS:HZ1	1.77	0.48
1:E:80:LEU:HG	1:E:84:SER:HB3	1.95	0.48
1:B:121:ILE:H	2:B:2001:GUN:HN9	1.61	0.48
1:D:75:LEU:HD11	1:D:94:THR:HG22	1.94	0.48
1:A:80:LEU:HD13	1:A:85:GLN:OE1	2.13	0.48
1:F:75:LEU:HD11	1:F:94:THR:HG22	1.95	0.47
1:A:119:PHE:CD1	1:A:135:LEU:HD13	2.50	0.47
1:D:24:LYS:CE	3:D:4034:HOH:O	2.60	0.47
1:C:33:TRP:CD1	1:C:36:ARG:HD3	2.50	0.47
1:F:163:HIS:HD2	3:F:5135:HOH:O	1.98	0.46
1:A:72:GLY:O	1:A:76:GLN:HG2	2.16	0.46
1:D:126:ASN:HD22	1:D:130:ASP:HB3	1.82	0.44
1:A:75:LEU:HD21	1:A:93:MET:O	2.17	0.44
1:D:159:SER:O	1:D:163:HIS:HD2	2.00	0.44
1:D:4:ASN:ND2	3:D:4108:HOH:O	2.46	0.44
1:B:86:GLU:HG3	3:B:2107:HOH:O	2.17	0.44
1:B:27:LEU:CD2	3:B:2122:HOH:O	2.40	0.44
1:A:63:ILE:CG1	1:B:27:LEU:HD13	2.40	0.44
1:A:39:LYS:HE3	1:A:39:LYS:HB2	1.82	0.44
1:D:165:ILE:HD12	1:D:165:ILE:HA	1.52	0.44
1:A:122:CYS:SG	1:A:125:LEU:HG	2.58	0.44
1:A:96:LEU:HB3	1:A:100:GLU:HB2	2.00	0.44
1:B:119:PHE:O	2:B:2001:GUN:H8	2.18	0.43
1:E:17:LEU:HD23	1:E:18:PHE:CE2	2.52	0.43
1:B:32:ILE:HD12	1:B:32:ILE:C	2.39	0.43
1:E:80:LEU:HD23	1:E:85:GLN:HA	2.01	0.43
1:A:36:ARG:NE	3:A:1059:HOH:O	2.51	0.43
1:A:123:ALA:H	2:A:1001:GUN:HN22	1.67	0.42
1:B:11:TYR:O	1:B:15:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:SER:O	1:C:163:HIS:HD2	2.03	0.42
1:D:106:ARG:NH1	3:D:4089:HOH:O	2.41	0.42
1:D:41:LEU:HD23	1:D:163:HIS:CE1	2.55	0.42
1:A:80:LEU:CD1	3:A:1067:HOH:O	2.67	0.42
1:D:114:ARG:HH11	1:D:114:ARG:HG3	1.85	0.41
1:E:123:ALA:H	2:E:6001:GUN:HN22	1.68	0.41
1:A:80:LEU:HD13	3:A:1067:HOH:O	2.20	0.41
1:C:108:ASN:O	1:C:112:LYS:HG3	2.20	0.41
1:A:53:HIS:CD2	3:A:1114:HOH:O	2.68	0.41
1:B:113:GLU:HB2	3:B:2104:HOH:O	2.21	0.41
1:B:27:LEU:O	1:B:27:LEU:HG	2.12	0.41
1:D:33:TRP:O	1:D:36:ARG:HD3	2.21	0.41
1:E:114:ARG:O	1:E:143:ARG:NH2	2.54	0.41
1:B:48:ILE:HD12	1:B:162:LEU:HD11	2.03	0.41
3:A:1010:HOH:O	1:B:56:PRO:HD3	2.21	0.40
1:C:165:ILE:O	1:C:167:LEU:HG	2.21	0.40
1:A:103:HIS:NE2	3:A:1063:HOH:O	2.37	0.40
1:B:121:ILE:O	2:B:2001:GUN:N3	2.54	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	163/174 (94%)	160 (98%)	2 (1%)	1 (1%)	28	13
1	B	162/174 (93%)	160 (99%)	2 (1%)	0	100	100
1	C	165/174 (95%)	163 (99%)	2 (1%)	0	100	100
1	D	162/174 (93%)	160 (99%)	2 (1%)	0	100	100
1	E	162/174 (93%)	159 (98%)	3 (2%)	0	100	100
1	F	166/174 (95%)	165 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	980/1044 (94%)	967 (99%)	12 (1%)	1 (0%)	55 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	LYS

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	145/154 (94%)	142 (98%)	3 (2%)	59 46
1	B	144/154 (94%)	138 (96%)	6 (4%)	34 17
1	C	147/154 (96%)	143 (97%)	4 (3%)	50 35
1	D	144/154 (94%)	142 (99%)	2 (1%)	71 64
1	E	144/154 (94%)	140 (97%)	4 (3%)	49 34
1	F	148/154 (96%)	147 (99%)	1 (1%)	87 84
All	All	872/924 (94%)	852 (98%)	20 (2%)	56 41

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

Mol	Chain	Res	Type
1	A	5	VAL
1	A	16	LYS
1	A	135	LEU
1	B	9	LEU
1	B	27	LEU
1	B	75	LEU
1	B	135	LEU
1	B	137	GLU
1	B	139	LEU
1	C	2	ASP
1	C	27	LEU

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Mol	Chain	Res	Type
1	C	128	LYS
1	C	135	LEU
1	D	9	LEU
1	D	165	ILE
1	E	27	LEU
1	E	80	LEU
1	E	135	LEU
1	E	139	LEU
1	F	135	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	20	ASN
1	A	53	HIS
1	A	126	ASN
1	B	20	ASN
1	C	4	ASN
1	C	20	ASN
1	C	126	ASN
1	C	163	HIS
1	D	20	ASN
1	D	126	ASN
1	D	163	HIS
1	E	4	ASN
1	E	20	ASN
1	E	126	ASN
1	E	163	HIS
1	F	4	ASN
1	F	20	ASN
1	F	126	ASN
1	F	163	HIS

5.3.3 RNA ⓘ

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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GUN	A	1001	-	9,12,12	1.51	1 (11%)	8,17,17	3.66	3 (37%)
2	GUN	B	2001	-	9,12,12	1.64	1 (11%)	8,17,17	3.82	4 (50%)
2	GUN	C	3001	-	9,12,12	1.68	1 (11%)	8,17,17	4.93	4 (50%)
2	GUN	D	4001	-	9,12,12	1.60	2 (22%)	8,17,17	4.06	4 (50%)
2	GUN	E	6001	-	9,12,12	1.71	1 (11%)	8,17,17	3.66	4 (50%)
2	GUN	F	5001	-	9,12,12	1.63	1 (11%)	8,17,17	4.92	7 (87%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GUN	A	1001	-	-	0/0/0/0	0/2/2/2
2	GUN	B	2001	-	-	0/0/0/0	0/2/2/2
2	GUN	C	3001	-	-	0/0/0/0	0/2/2/2
2	GUN	D	4001	-	-	0/0/0/0	0/2/2/2
2	GUN	E	6001	-	-	0/0/0/0	0/2/2/2
2	GUN	F	5001	-	-	0/0/0/0	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4001	GUN	C4-N9	2.09	1.38	1.34
2	A	1001	GUN	C6-N1	3.77	1.39	1.33
2	D	4001	GUN	C6-N1	3.81	1.39	1.33
2	B	2001	GUN	C6-N1	3.95	1.40	1.33
2	E	6001	GUN	C6-N1	4.30	1.40	1.33
2	C	3001	GUN	C6-N1	4.39	1.41	1.33
2	F	5001	GUN	C6-N1	4.45	1.41	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3001	GUN	C5-C6-N1	-9.40	110.10	123.48
2	F	5001	GUN	C5-C6-N1	-8.74	111.04	123.48
2	D	4001	GUN	C5-C6-N1	-8.43	111.47	123.48
2	B	2001	GUN	C5-C6-N1	-8.26	111.72	123.48
2	A	1001	GUN	C5-C6-N1	-7.91	112.22	123.48
2	E	6001	GUN	C5-C6-N1	-7.75	112.45	123.48
2	C	3001	GUN	C2-N3-C4	-5.51	108.72	115.16
2	F	5001	GUN	C2-N3-C4	-5.27	109.01	115.16
2	A	1001	GUN	C2-N3-C4	-2.98	111.67	115.16
2	B	2001	GUN	C2-N3-C4	-2.63	112.09	115.16
2	E	6001	GUN	N3-C2-N1	-2.57	123.71	127.46
2	D	4001	GUN	C2-N3-C4	-2.47	112.27	115.16
2	D	4001	GUN	N3-C2-N1	-2.46	123.86	127.46
2	E	6001	GUN	C2-N3-C4	-2.27	112.51	115.16
2	F	5001	GUN	N2-C2-N1	-2.16	113.79	117.24
2	B	2001	GUN	N3-C2-N1	-2.15	124.32	127.46
2	F	5001	GUN	N3-C2-N1	-2.10	124.40	127.46
2	F	5001	GUN	N2-C2-N3	2.20	121.81	117.75
2	C	3001	GUN	C4-C5-N7	3.26	112.56	109.41
2	F	5001	GUN	C4-C5-N7	4.79	114.03	109.41
2	A	1001	GUN	C6-N1-C2	5.42	123.85	116.06
2	E	6001	GUN	C6-N1-C2	5.47	123.92	116.06
2	B	2001	GUN	C6-N1-C2	5.72	124.29	116.06
2	D	4001	GUN	C6-N1-C2	6.29	125.10	116.06
2	F	5001	GUN	C6-N1-C2	7.00	126.12	116.06
2	C	3001	GUN	C6-N1-C2	7.39	126.70	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	GUN	3	0
2	B	2001	GUN	4	0
2	C	3001	GUN	1	0
2	D	4001	GUN	2	0
2	E	6001	GUN	3	0
2	F	5001	GUN	1	0

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	165/174 (94%)	0.34	8 (4%) 31 26	15, 24, 33, 35	0
1	B	164/174 (94%)	0.11	3 (1%) 69 65	15, 23, 32, 35	0
1	C	167/174 (95%)	0.21	3 (1%) 69 65	13, 21, 32, 43	0
1	D	164/174 (94%)	0.15	3 (1%) 69 65	13, 23, 32, 37	0
1	E	164/174 (94%)	0.31	6 (3%) 42 37	15, 24, 33, 35	0
1	F	168/174 (96%)	0.31	1 (0%) 89 87	12, 21, 30, 32	0
All	All	992/1044 (95%)	0.24	24 (2%) 59 55	12, 23, 32, 43	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	73	ARG	3.9
1	E	75	LEU	3.5
1	A	73	ARG	3.1
1	A	77	SER	3.0
1	A	86	GLU	2.7
1	A	97	ASP	2.7
1	E	142	ARG	2.6
1	C	167	LEU	2.5
1	C	76	GLN	2.5
1	F	73	ARG	2.4
1	E	77	SER	2.4
1	A	102	VAL	2.4
1	A	95	THR	2.3
1	A	127	ASN	2.2
1	E	99	ALA	2.2
1	A	163	HIS	2.1
1	D	73	ARG	2.1
1	D	142	ARG	2.1
1	C	148	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	27	LEU	2.1
1	E	134	GLN	2.1
1	B	142	ARG	2.0
1	D	133	ARG	2.0
1	B	81	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GUN	C	3001	11/11	0.76	0.22	8.78	24,24,25,25	0
2	GUN	F	5001	11/11	0.85	0.17	3.77	23,23,24,25	0
2	GUN	E	6001	11/11	0.94	0.14	1.35	25,25,25,25	0
2	GUN	B	2001	11/11	0.93	0.11	0.32	22,23,23,23	0
2	GUN	A	1001	11/11	0.93	0.13	0.01	24,25,25,25	0
2	GUN	D	4001	11/11	0.94	0.10	-0.43	22,22,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.