



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:32 am BST

PDB ID : 2MCP
Title : REFINED CRYSTAL STRUCTURE OF THE MC/PC603 FAB-PHOSPHOCHOLINE COMPLEX AT 3.1 ANGSTROMS RESOLUTION
Authors : Padlan, E.A.; Cohen, G.H.; Davies, D.R.
Deposited on : 1984-10-15
Resolution : 3.10 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

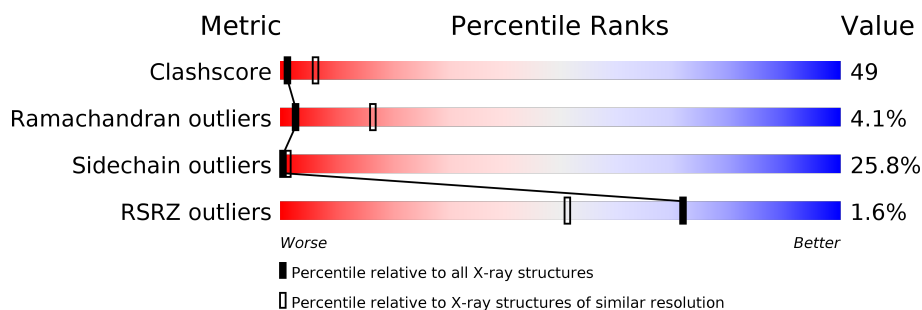
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	220	<div> <div>2%</div> <div> <div></div> <div>32%</div> <div>46%</div> <div>18%</div> <div>.</div> </div> </div>
2	H	222	<div> <div></div> <div> <div>36%</div> <div>45%</div> <div>17%</div> <div>.</div> </div> </div>

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
3	PC	H	223	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3412 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 IGA-KAPPA MCP C603 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	220	Total	C	N	O	S	0	0	0
			1692	1048	286	350	8			

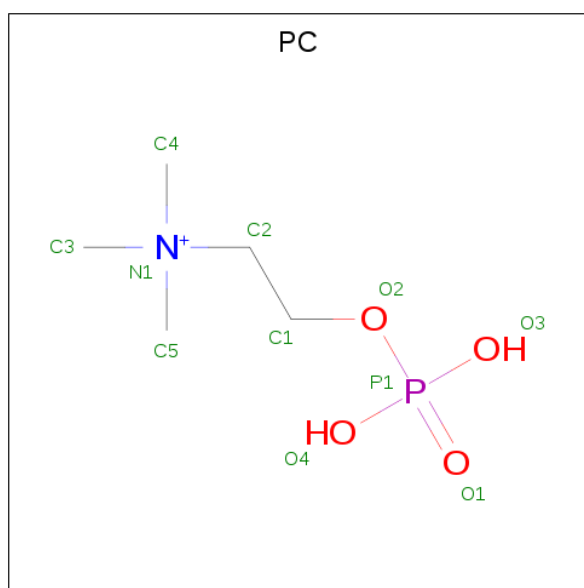
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	112	ILE	LEU	CONFLICT	GB 208622

- Molecule 2 is a protein called IGA-KAPPA MCP C603 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1709	1079	286	334	10			

- Molecule 3 is PHOSPHOCHOLINE (three-letter code: PC) (formula: $C_5H_{15}NO_4P$).

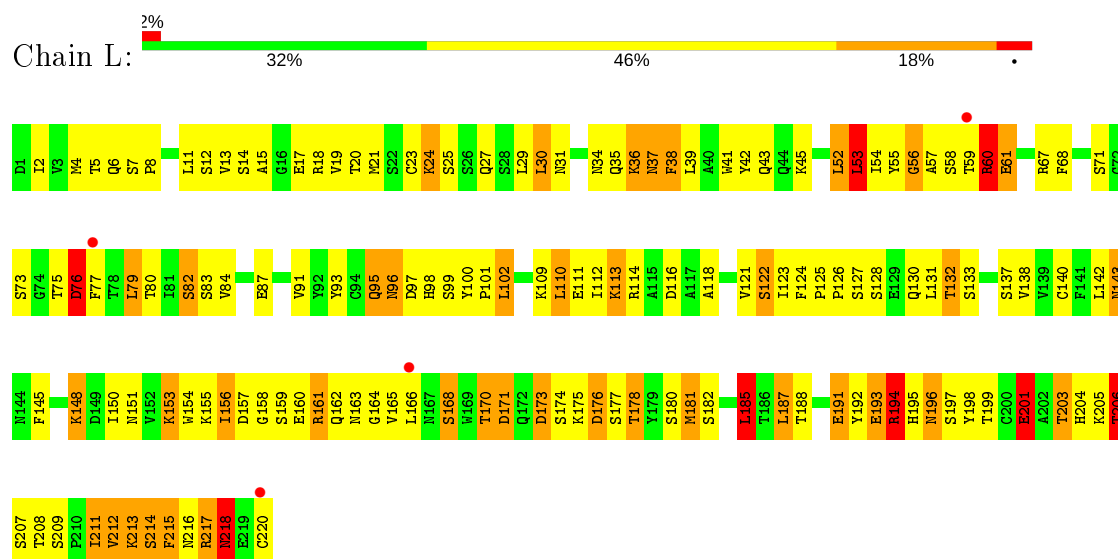


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	N	O	P	0	0
			11	5	1	4	1		

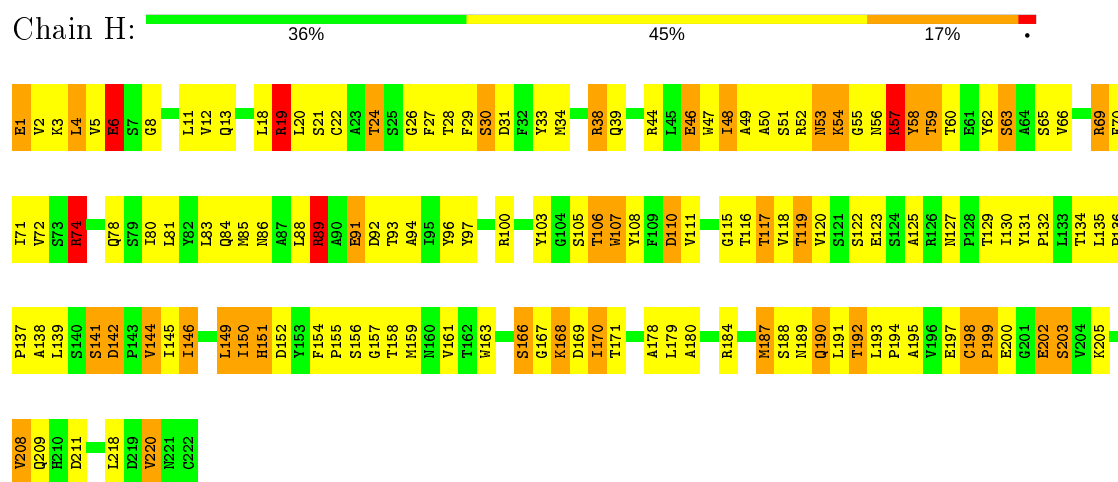
3 Residue-property plots

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: IGA-KAPPA MCPC603 FAB (LIGHT CHAIN)



• Molecule 2: IGA-KAPPA MCPC603 FAB (HEAVY CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	162.53 Å 162.53 Å 60.72 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.10 7.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10) 51.1 (7.99-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.185 , (Not available) 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 9.1	EDS
L-test for twinning ¹	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.150 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3412	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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

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

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	L	0.93	1/1728 (0.1%)	1.54	19/2344 (0.8%)
2	H	0.93	0/1753	1.56	14/2389 (0.6%)
All	All	0.93	1/3481 (0.0%)	1.55	33/4733 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	56	GLY	N-CA	6.42	1.55	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	19	ARG	NE-CZ-NH1	12.73	126.67	120.30
2	H	69	ARG	NE-CZ-NH1	9.81	125.20	120.30
2	H	19	ARG	NE-CZ-NH2	-9.27	115.67	120.30
2	H	89	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	L	60	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	L	56	GLY	N-CA-C	-7.61	94.07	113.10
1	L	76	ASP	CB-CG-OD1	7.54	125.09	118.30
1	L	194	ARG	NE-CZ-NH1	7.29	123.95	120.30
2	H	69	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	L	173	ASP	CB-CG-OD1	6.49	124.14	118.30
1	L	67	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	H	97	TYR	CA-CB-CG	6.08	124.94	113.40
2	H	74	ARG	CA-CB-CG	5.95	126.49	113.40
1	L	60	ARG	CD-NE-CZ	5.91	131.87	123.60
2	H	149	LEU	CA-CB-CG	5.90	128.86	115.30
2	H	151	HIS	N-CA-C	5.89	126.90	111.00
2	H	4	LEU	CA-CB-CG	5.86	128.79	115.30
1	L	97	ASP	CB-CG-OD1	5.68	123.41	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	158	GLY	N-CA-C	-5.63	99.04	113.10
2	H	44	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	H	150	ILE	CB-CA-C	5.61	122.82	111.60
2	H	107	TRP	CA-CB-CG	5.61	124.35	113.70
1	L	58	SER	N-CA-CB	-5.54	102.19	110.50
1	L	56	GLY	CA-C-O	-5.54	110.63	120.60
1	L	53	LEU	CB-CA-C	5.43	120.53	110.20
1	L	185	LEU	CA-CB-CG	5.43	127.78	115.30
1	L	212	VAL	N-CA-C	5.34	125.42	111.00
1	L	211	ILE	CB-CA-C	5.22	122.03	111.60
1	L	61	GLU	CG-CD-OE1	5.21	128.73	118.30
1	L	201	GLU	CA-CB-CG	5.19	124.82	113.40
1	L	191	GLU	CG-CD-OE1	5.12	128.53	118.30
1	L	217	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	H	6	GLU	CG-CD-OE1	5.08	128.47	118.30

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	L	1692	0	1622	184	8
2	H	1709	0	1648	158	8
3	H	11	0	13	7	0
All	All	3412	0	3283	331	8

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 49.

All (331) 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:L:153:LYS:HD2	1:L:161:ARG:HG2	1.23	1.17
1:L:201:GLU:HB3	1:L:212:VAL:HG22	1.31	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:223:PC:H22	3:H:223:PC:O1	1.53	1.08
2:H:49:ALA:HB1	2:H:72:VAL:HG21	1.38	1.02
2:H:49:ALA:CB	2:H:72:VAL:HG21	1.93	0.98
2:H:136:PRO:HD2	2:H:139:LEU:HD12	1.42	0.98
1:L:199:THR:HG22	1:L:214:SER:HB2	1.45	0.97
1:L:198:TYR:HB2	1:L:215:PHE:CE2	2.03	0.93
2:H:54:LYS:HB2	2:H:58:TYR:CZ	2.04	0.91
1:L:187:LEU:HD13	1:L:192:TYR:HB2	1.51	0.89
1:L:195:HIS:O	1:L:218:ASN:ND2	2.06	0.88
2:H:11:LEU:HD13	2:H:155:PRO:HG3	1.56	0.86
2:H:52:ARG:HE	2:H:59:THR:HG22	1.39	0.86
1:L:31:ASN:HD22	1:L:34:ASN:HB2	1.38	0.86
2:H:24:THR:HG21	2:H:29:PHE:CD1	2.11	0.85
2:H:54:LYS:HB2	2:H:58:TYR:OH	1.78	0.83
2:H:159:MET:SD	2:H:208:VAL:HG12	2.19	0.83
1:L:153:LYS:CD	1:L:161:ARG:HG2	2.05	0.82
1:L:157:ASP:CG	1:L:195:HIS:HB3	1.98	0.82
2:H:4:LEU:HD22	2:H:24:THR:OG1	1.79	0.82
2:H:159:MET:HG2	2:H:187:MET:HE2	1.63	0.81
1:L:201:GLU:CB	1:L:212:VAL:HG22	2.08	0.81
1:L:100:TYR:CZ	3:H:223:PC:H43	2.15	0.81
2:H:24:THR:HG21	2:H:29:PHE:HD1	1.45	0.81
1:L:96:ASN:ND2	1:L:98:HIS:H	1.79	0.80
2:H:88:LEU:HD13	2:H:120:VAL:HG22	1.63	0.79
1:L:60:ARG:HB2	1:L:60:ARG:HH21	1.45	0.79
2:H:202:GLU:OE1	2:H:202:GLU:HA	1.80	0.79
1:L:157:ASP:CB	1:L:195:HIS:HB3	2.15	0.77
2:H:145:ILE:HD13	2:H:192:THR:HB	1.65	0.77
1:L:130:GLN:HE22	1:L:137:SER:HB2	1.50	0.76
2:H:193:LEU:HD12	2:H:197:GLU:HB3	1.67	0.76
2:H:88:LEU:HD13	2:H:120:VAL:CG2	2.15	0.76
1:L:162:GLN:HG3	1:L:163:ASN:H	1.50	0.76
2:H:38:ARG:HG2	2:H:48:ILE:HG21	1.68	0.75
1:L:151:ASN:OD1	1:L:203:THR:HG22	1.84	0.75
2:H:48:ILE:HG13	2:H:49:ALA:H	1.52	0.75
1:L:196:ASN:O	1:L:216:ASN:HA	1.87	0.75
1:L:101:PRO:HB3	2:H:47:TRP:CZ3	2.22	0.74
2:H:145:ILE:HG23	2:H:190:GLN:HE21	1.52	0.73
1:L:157:ASP:HB2	1:L:195:HIS:HB3	1.69	0.73
2:H:52:ARG:NE	2:H:59:THR:HG22	2.02	0.73
2:H:159:MET:HG2	2:H:187:MET:CE	2.19	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:146:ILE:HD11	2:H:220:VAL:HB	1.71	0.72
3:H:223:PC:O1	3:H:223:PC:C2	2.26	0.71
1:L:191:GLU:HG3	1:L:194:ARG:NH1	2.04	0.71
2:H:93:THR:HG23	2:H:119:THR:HA	1.71	0.70
2:H:88:LEU:HB3	2:H:120:VAL:HG21	1.72	0.70
2:H:12:VAL:HG21	2:H:18:LEU:CG	2.21	0.70
2:H:62:TYR:HE1	2:H:72:VAL:HG23	1.57	0.70
1:L:84:VAL:HG12	1:L:112:ILE:HD11	1.73	0.70
2:H:31:ASP:HA	2:H:53:ASN:HB2	1.74	0.70
2:H:171:THR:HB	2:H:192:THR:HG23	1.75	0.69
2:H:117:THR:HG21	2:H:157:GLY:HA2	1.73	0.69
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.75	0.69
1:L:60:ARG:HH21	1:L:60:ARG:CB	2.04	0.69
2:H:93:THR:HG23	2:H:118:VAL:O	1.92	0.68
2:H:145:ILE:HG23	2:H:190:GLN:NE2	2.08	0.68
1:L:193:GLU:C	1:L:218:ASN:HD21	1.96	0.68
2:H:169:ASP:CG	2:H:194:PRO:HD3	2.15	0.67
2:H:66:VAL:CG1	2:H:70:PHE:HB2	2.24	0.67
2:H:198:CYS:N	2:H:199:PRO:HD3	2.08	0.67
1:L:34:ASN:HB2	1:L:36:LYS:HZ3	1.59	0.67
1:L:100:TYR:CD2	1:L:102:LEU:HD13	2.30	0.67
1:L:24:LYS:HA	1:L:75:THR:O	1.94	0.67
2:H:170:ILE:CG2	2:H:191:LEU:HD11	2.25	0.67
1:L:100:TYR:CE1	3:H:223:PC:H43	2.30	0.67
1:L:8:PRO:HG2	1:L:11:LEU:HG	1.77	0.67
1:L:19:VAL:O	1:L:80:THR:HG23	1.96	0.66
2:H:12:VAL:HG21	2:H:18:LEU:CD1	2.25	0.66
1:L:153:LYS:HZ2	1:L:161:ARG:HD3	1.58	0.66
2:H:34:MET:HB3	2:H:81:LEU:HD22	1.77	0.66
1:L:96:ASN:HD22	1:L:98:HIS:H	1.40	0.66
1:L:37:ASN:HD22	1:L:57:ALA:HB2	1.59	0.65
2:H:72:VAL:HG22	2:H:83:LEU:HD12	1.77	0.65
2:H:149:LEU:HD13	2:H:151:HIS:HB2	1.77	0.65
1:L:142:LEU:HD13	1:L:181:MET:HG2	1.79	0.65
1:L:187:LEU:CD1	1:L:192:TYR:HB2	2.27	0.64
2:H:12:VAL:HG21	2:H:18:LEU:HD11	1.80	0.63
1:L:201:GLU:HA	1:L:211:ILE:O	1.99	0.63
1:L:170:THR:HG23	1:L:171:ASP:O	1.99	0.63
2:H:103:TYR:HB2	2:H:107:TRP:CE3	2.33	0.63
1:L:31:ASN:ND2	1:L:36:LYS:HZ3	1.96	0.63
2:H:57:LYS:O	2:H:59:THR:N	2.25	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:135:LEU:HD22	2:H:139:LEU:HB2	1.81	0.62
2:H:130:ILE:CD1	2:H:208:VAL:HG21	2.29	0.62
2:H:166:SER:C	2:H:170:ILE:HD13	2.20	0.62
2:H:107:TRP:CZ2	3:H:223:PC:H33	2.35	0.62
1:L:161:ARG:O	1:L:162:GLN:HB2	1.98	0.62
1:L:193:GLU:HA	1:L:218:ASN:ND2	2.15	0.62
2:H:20:LEU:HD22	2:H:116:THR:HG21	1.80	0.62
2:H:38:ARG:HD2	2:H:46:GLU:HG2	1.82	0.61
2:H:167:GLY:N	2:H:170:ILE:HD13	2.15	0.61
2:H:169:ASP:O	2:H:170:ILE:HG13	2.01	0.61
1:L:84:VAL:CG1	1:L:112:ILE:HD11	2.30	0.61
2:H:131:TYR:HD2	2:H:149:LEU:HD12	1.66	0.61
1:L:31:ASN:ND2	1:L:34:ASN:HB2	2.13	0.61
1:L:29:LEU:HD13	1:L:39:LEU:HB2	1.83	0.60
2:H:2:VAL:HG12	2:H:111:VAL:HG21	1.83	0.60
1:L:60:ARG:NH2	1:L:60:ARG:HB2	2.14	0.60
1:L:155:LYS:HG2	1:L:160:GLU:O	2.02	0.60
1:L:191:GLU:HA	1:L:194:ARG:NH1	2.15	0.60
1:L:166:LEU:HD23	2:H:178:ALA:HB1	1.84	0.60
1:L:145:PHE:CZ	1:L:150:ILE:HG21	2.38	0.59
2:H:69:ARG:O	2:H:86:ASN:HB2	2.02	0.59
1:L:122:SER:O	1:L:140:CYS:HA	2.03	0.59
2:H:136:PRO:HD2	2:H:139:LEU:CD1	2.25	0.59
1:L:157:ASP:HB2	1:L:195:HIS:CB	2.32	0.58
1:L:60:ARG:CG	1:L:60:ARG:HH21	2.16	0.58
1:L:60:ARG:NH2	1:L:68:PHE:O	2.36	0.58
2:H:66:VAL:HG13	2:H:70:PHE:HB2	1.84	0.58
1:L:42:TYR:CE1	1:L:95:GLN:NE2	2.71	0.58
2:H:136:PRO:O	2:H:138:ALA:N	2.35	0.58
2:H:130:ILE:HD11	2:H:208:VAL:HG21	1.84	0.58
1:L:42:TYR:HE1	1:L:95:GLN:NE2	2.01	0.58
1:L:150:ILE:HG23	1:L:150:ILE:O	2.04	0.58
1:L:162:GLN:HG2	1:L:164:GLY:H	1.69	0.58
1:L:39:LEU:HD13	1:L:77:PHE:CD1	2.38	0.58
1:L:37:ASN:ND2	1:L:77:PHE:HE2	2.01	0.58
1:L:143:ASN:ND2	2:H:190:GLN:OE1	2.30	0.57
1:L:31:ASN:HD22	1:L:36:LYS:HZ3	1.50	0.57
1:L:55:TYR:CE2	1:L:59:THR:HG21	2.39	0.57
1:L:20:THR:HG23	1:L:80:THR:OG1	2.04	0.57
2:H:88:LEU:CD1	2:H:120:VAL:HG22	2.35	0.56
1:L:34:ASN:HB2	1:L:36:LYS:NZ	2.19	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:CYS:N	2:H:81:LEU:O	2.39	0.56
1:L:101:PRO:HB3	2:H:47:TRP:HZ3	1.71	0.56
1:L:96:ASN:HD21	1:L:99:SER:H	1.53	0.56
1:L:159:SER:O	1:L:160:GLU:HG2	2.05	0.56
2:H:70:PHE:HA	2:H:84:GLN:O	2.06	0.56
1:L:29:LEU:HD12	1:L:77:PHE:CE1	2.41	0.56
2:H:130:ILE:CD1	2:H:150:ILE:HG23	2.36	0.56
2:H:28:THR:HG22	2:H:31:ASP:OD1	2.05	0.56
2:H:53:ASN:O	2:H:55:GLY:N	2.34	0.56
2:H:66:VAL:HG13	2:H:70:PHE:CG	2.41	0.56
1:L:35:GLN:C	1:L:36:LYS:HG3	2.25	0.56
1:L:30:LEU:HG	1:L:31:ASN:O	2.06	0.55
2:H:31:ASP:HA	2:H:53:ASN:CB	2.36	0.55
1:L:201:GLU:HB3	1:L:212:VAL:CG2	2.22	0.55
1:L:118:ALA:HA	1:L:206:THR:HG21	1.87	0.55
1:L:96:ASN:ND2	1:L:98:HIS:HB3	2.21	0.55
1:L:191:GLU:HG3	1:L:194:ARG:HH12	1.69	0.55
1:L:124:PHE:HZ	2:H:145:ILE:CG2	2.20	0.55
1:L:37:ASN:ND2	1:L:73:SER:HA	2.22	0.55
1:L:124:PHE:HZ	2:H:145:ILE:HG22	1.71	0.55
1:L:153:LYS:NZ	1:L:161:ARG:HG2	2.22	0.54
1:L:60:ARG:NH2	1:L:60:ARG:CB	2.69	0.54
2:H:11:LEU:HD11	2:H:154:PHE:HE2	1.73	0.54
1:L:162:GLN:CG	1:L:163:ASN:H	2.19	0.54
1:L:145:PHE:HE1	1:L:148:LYS:O	1.91	0.54
1:L:34:ASN:HB2	1:L:36:LYS:HE2	1.90	0.54
2:H:4:LEU:CD2	2:H:24:THR:OG1	2.54	0.54
1:L:31:ASN:HB3	1:L:35:GLN:H	1.72	0.53
1:L:191:GLU:HA	1:L:194:ARG:HH11	1.72	0.53
1:L:162:GLN:CG	1:L:163:ASN:N	2.71	0.53
1:L:17:GLU:O	1:L:83:SER:HA	2.09	0.53
1:L:96:ASN:ND2	1:L:98:HIS:N	2.54	0.53
2:H:138:ALA:O	2:H:139:LEU:HD23	2.08	0.53
1:L:212:VAL:O	1:L:212:VAL:HG12	2.09	0.53
1:L:38:PHE:CD2	2:H:107:TRP:HD1	2.27	0.53
1:L:54:ILE:HD13	1:L:60:ARG:HA	1.91	0.53
2:H:93:THR:CG2	2:H:119:THR:HA	2.36	0.53
2:H:96:TYR:O	2:H:115:GLY:HA2	2.09	0.53
1:L:30:LEU:HA	1:L:37:ASN:HA	1.91	0.52
2:H:152:ASP:OD1	2:H:184:ARG:NH1	2.42	0.52
2:H:38:ARG:HG3	2:H:46:GLU:HG2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:160:GLU:O	1:L:161:ARG:HD2	2.10	0.52
1:L:37:ASN:HD21	1:L:73:SER:HA	1.75	0.52
2:H:8:GLY:O	2:H:20:LEU:HD23	2.10	0.52
1:L:153:LYS:HZ2	1:L:161:ARG:CD	2.23	0.52
2:H:135:LEU:HD22	2:H:139:LEU:CB	2.40	0.52
1:L:34:ASN:HB2	1:L:36:LYS:CE	2.40	0.52
1:L:13:VAL:O	1:L:112:ILE:HA	2.09	0.52
1:L:162:GLN:HG3	1:L:163:ASN:N	2.23	0.52
1:L:176:ASP:OD2	1:L:178:THR:OG1	2.28	0.52
2:H:69:ARG:NH2	2:H:92:ASP:OD1	2.43	0.51
1:L:193:GLU:HA	1:L:218:ASN:CG	2.31	0.51
1:L:124:PHE:CE1	2:H:135:LEU:HG	2.46	0.51
1:L:20:THR:OG1	1:L:80:THR:HG23	2.10	0.51
2:H:20:LEU:CD2	2:H:116:THR:HG21	2.41	0.51
2:H:49:ALA:CB	2:H:72:VAL:CG2	2.80	0.51
2:H:130:ILE:HD13	2:H:150:ILE:HG23	1.92	0.51
2:H:29:PHE:CE2	2:H:74:ARG:HD3	2.45	0.51
2:H:6:GLU:HG3	2:H:116:THR:HG22	1.93	0.50
1:L:35:GLN:O	1:L:36:LYS:HG3	2.11	0.50
2:H:6:GLU:HA	2:H:21:SER:O	2.11	0.50
2:H:85:MET:HB3	2:H:88:LEU:HD21	1.93	0.50
1:L:124:PHE:CZ	2:H:145:ILE:HG22	2.45	0.50
1:L:153:LYS:NZ	1:L:161:ARG:CG	2.74	0.50
2:H:161:VAL:HG11	2:H:189:ASN:ND2	2.27	0.50
2:H:144:VAL:CG2	2:H:195:ALA:HA	2.42	0.50
1:L:116:ASP:OD2	1:L:205:LYS:HE2	2.12	0.50
1:L:127:SER:O	1:L:131:LEU:HG	2.12	0.50
1:L:173:ASP:OD2	1:L:175:LYS:N	2.44	0.50
1:L:114:ARG:HD2	1:L:176:ASP:O	2.12	0.50
2:H:161:VAL:HG21	2:H:187:MET:HE3	1.93	0.49
1:L:2:ILE:CG2	1:L:96:ASN:OD1	2.60	0.49
1:L:204:HIS:HB3	1:L:206:THR:OG1	2.11	0.49
1:L:101:PRO:HB3	2:H:47:TRP:CE3	2.48	0.49
1:L:160:GLU:O	1:L:161:ARG:HG3	2.11	0.49
2:H:50:ALA:O	2:H:60:THR:HA	2.13	0.49
1:L:13:VAL:HG21	1:L:84:VAL:HG21	1.95	0.49
2:H:100:ARG:HD3	2:H:110:ASP:OD1	2.12	0.49
1:L:12:SER:OG	1:L:113:LYS:HD3	2.11	0.49
1:L:13:VAL:HG23	1:L:112:ILE:HD13	1.94	0.49
1:L:24:LYS:HD3	1:L:76:ASP:OD1	2.13	0.49
1:L:121:VAL:O	1:L:213:LYS:HD2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:130:GLN:NE2	1:L:137:SER:HB2	2.24	0.49
2:H:12:VAL:CG2	2:H:18:LEU:HD11	2.42	0.48
1:L:153:LYS:HZ3	1:L:161:ARG:CG	2.27	0.48
1:L:154:TRP:O	1:L:161:ARG:HA	2.12	0.48
2:H:107:TRP:CE2	3:H:223:PC:H33	2.49	0.48
1:L:188:THR:OG1	1:L:191:GLU:HB2	2.13	0.48
1:L:15:ALA:HB2	1:L:112:ILE:HD12	1.95	0.48
1:L:195:HIS:CD2	1:L:195:HIS:H	2.31	0.48
1:L:31:ASN:ND2	1:L:36:LYS:NZ	2.62	0.48
1:L:160:GLU:O	1:L:161:ARG:CG	2.62	0.48
2:H:202:GLU:O	2:H:203:SER:CB	2.62	0.47
2:H:29:PHE:CZ	2:H:74:ARG:HD3	2.49	0.47
1:L:55:TYR:C	1:L:56:GLY:O	2.44	0.47
1:L:166:LEU:HD23	2:H:178:ALA:CB	2.43	0.47
2:H:24:THR:HG22	2:H:24:THR:O	2.14	0.47
2:H:53:ASN:C	2:H:55:GLY:N	2.67	0.47
2:H:12:VAL:O	2:H:120:VAL:HA	2.15	0.47
2:H:169:ASP:OD2	2:H:194:PRO:HD3	2.15	0.47
2:H:24:THR:HG23	2:H:27:PHE:CZ	2.50	0.47
2:H:39:GLN:C	2:H:94:ALA:HB1	2.34	0.47
1:L:193:GLU:HA	1:L:218:ASN:OD1	2.13	0.47
2:H:48:ILE:HA	2:H:63:SER:HB3	1.97	0.47
2:H:31:ASP:C	2:H:53:ASN:HB3	2.35	0.47
2:H:54:LYS:O	2:H:54:LYS:HD2	2.14	0.47
1:L:192:TYR:O	1:L:198:TYR:OH	2.32	0.47
1:L:173:ASP:OD2	1:L:173:ASP:C	2.53	0.47
2:H:141:SER:O	2:H:142:ASP:HB3	2.15	0.47
2:H:130:ILE:HG22	2:H:218:LEU:HD22	1.97	0.46
2:H:161:VAL:HG11	2:H:189:ASN:HD22	1.80	0.46
1:L:181:MET:HG3	1:L:182:SER:N	2.30	0.46
2:H:38:ARG:CG	2:H:46:GLU:HG2	2.45	0.46
1:L:52:LEU:HD13	1:L:61:GLU:HB2	1.97	0.46
2:H:150:ILE:HG21	2:H:208:VAL:HG11	1.97	0.46
2:H:1:GLU:O	2:H:26:GLY:HA3	2.16	0.46
1:L:31:ASN:HD22	1:L:36:LYS:NZ	2.13	0.46
1:L:25:SER:O	1:L:75:THR:HB	2.16	0.46
2:H:205:LYS:HA	2:H:218:LEU:O	2.15	0.46
1:L:14:SER:O	1:L:15:ALA:HB3	2.16	0.46
1:L:43:GLN:HB2	1:L:53:LEU:HG	1.97	0.46
2:H:103:TYR:HA	2:H:106:THR:O	2.16	0.46
2:H:145:ILE:CG2	2:H:190:GLN:NE2	2.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:24:LYS:CA	1:L:75:THR:O	2.61	0.45
1:L:42:TYR:HE1	1:L:95:GLN:HE21	1.63	0.45
1:L:160:GLU:O	1:L:161:ARG:CD	2.65	0.45
1:L:153:LYS:HZ3	1:L:161:ARG:CB	2.29	0.45
2:H:198:CYS:N	2:H:199:PRO:CD	2.77	0.45
1:L:153:LYS:HD2	1:L:161:ARG:CG	2.17	0.45
2:H:135:LEU:HD22	2:H:139:LEU:CD1	2.47	0.45
2:H:24:THR:CG2	2:H:29:PHE:HB2	2.47	0.45
1:L:38:PHE:N	1:L:38:PHE:CD1	2.84	0.45
1:L:37:ASN:ND2	1:L:57:ALA:HB2	2.30	0.45
1:L:193:GLU:HA	1:L:218:ASN:HD21	1.82	0.45
2:H:170:ILE:HG22	2:H:191:LEU:HD11	1.99	0.44
2:H:38:ARG:HG2	2:H:48:ILE:CG2	2.43	0.44
1:L:19:VAL:O	1:L:80:THR:HA	2.17	0.44
2:H:100:ARG:CD	2:H:110:ASP:OD1	2.64	0.44
1:L:39:LEU:C	1:L:39:LEU:HD23	2.38	0.44
1:L:95:GLN:HG2	1:L:96:ASN:N	2.30	0.44
2:H:132:PRO:CB	2:H:220:VAL:HG13	2.47	0.44
2:H:57:LYS:N	2:H:57:LYS:HD3	2.31	0.44
1:L:91:VAL:HG22	1:L:109:LYS:HG2	2.00	0.44
1:L:126:PRO:HG3	1:L:138:VAL:HG22	1.99	0.44
2:H:169:ASP:O	2:H:170:ILE:CG1	2.65	0.44
1:L:19:VAL:O	1:L:80:THR:CG2	2.65	0.44
1:L:197:SER:HA	1:L:216:ASN:HB3	1.99	0.44
2:H:163:TRP:HE1	2:H:189:ASN:ND2	2.15	0.44
1:L:130:GLN:HB2	2:H:131:TYR:CZ	2.53	0.44
2:H:125:ALA:HA	2:H:154:PHE:O	2.18	0.44
2:H:161:VAL:CG2	2:H:187:MET:HE3	2.48	0.44
2:H:200:GLU:C	2:H:202:GLU:N	2.71	0.44
2:H:29:PHE:O	2:H:31:ASP:N	2.49	0.44
1:L:162:GLN:HG2	1:L:164:GLY:N	2.33	0.44
1:L:96:ASN:C	1:L:96:ASN:ND2	2.71	0.44
2:H:33:TYR:CE1	3:H:223:PC:H32	2.53	0.43
1:L:153:LYS:HZ3	1:L:161:ARG:HG2	1.83	0.43
1:L:168:SER:O	1:L:181:MET:HA	2.18	0.43
1:L:18:ARG:HB2	1:L:82:SER:O	2.18	0.43
1:L:38:PHE:HD1	1:L:38:PHE:N	2.15	0.43
2:H:89:ARG:HE	2:H:91:GLU:CD	2.21	0.43
1:L:193:GLU:CA	1:L:218:ASN:HD21	2.31	0.43
1:L:199:THR:HG22	1:L:214:SER:CB	2.32	0.43
1:L:6:GLN:OE1	1:L:93:TYR:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:7:SER:HA	1:L:8:PRO:C	2.39	0.43
1:L:96:ASN:ND2	1:L:98:HIS:CB	2.82	0.43
1:L:156:ILE:O	1:L:197:SER:O	2.36	0.43
2:H:169:ASP:OD2	2:H:194:PRO:CD	2.67	0.43
2:H:130:ILE:HD12	2:H:208:VAL:HG21	2.00	0.43
2:H:29:PHE:C	2:H:31:ASP:H	2.21	0.43
2:H:135:LEU:HA	2:H:136:PRO:HD3	1.84	0.42
2:H:38:ARG:CD	2:H:46:GLU:HG2	2.47	0.42
1:L:41:TRP:CE3	1:L:79:LEU:HD12	2.54	0.42
2:H:66:VAL:HG13	2:H:70:PHE:CB	2.48	0.42
1:L:130:GLN:HB2	2:H:131:TYR:CE2	2.54	0.42
1:L:128:SER:O	1:L:132:THR:HG22	2.19	0.42
1:L:145:PHE:CE1	1:L:150:ILE:HG21	2.54	0.42
1:L:173:ASP:OD2	1:L:174:SER:N	2.52	0.42
1:L:198:TYR:HB2	1:L:215:PHE:CD2	2.51	0.42
1:L:110:LEU:C	1:L:110:LEU:HD12	2.40	0.42
1:L:2:ILE:HG23	1:L:96:ASN:OD1	2.19	0.42
1:L:31:ASN:HD22	1:L:36:LYS:CE	2.32	0.42
2:H:62:TYR:CE1	2:H:72:VAL:HG23	2.47	0.42
2:H:103:TYR:HB2	2:H:107:TRP:CD2	2.55	0.42
1:L:29:LEU:HD12	1:L:77:PHE:CZ	2.54	0.42
2:H:69:ARG:HH22	2:H:92:ASP:CG	2.23	0.42
2:H:163:TRP:HE1	2:H:189:ASN:HD21	1.68	0.41
2:H:157:GLY:HA3	2:H:211:ASP:OD2	2.19	0.41
1:L:153:LYS:HA	1:L:153:LYS:HD3	1.89	0.41
2:H:163:TRP:HE1	2:H:189:ASN:CG	2.24	0.41
2:H:145:ILE:CD1	2:H:192:THR:HB	2.42	0.41
2:H:56:ASN:C	2:H:57:LYS:HG2	2.40	0.41
1:L:125:PRO:HA	1:L:126:PRO:HD3	1.94	0.41
1:L:165:VAL:HG23	1:L:185:LEU:HD23	2.01	0.41
2:H:193:LEU:HB2	2:H:194:PRO:HD2	2.02	0.41
1:L:2:ILE:HG21	1:L:96:ASN:OD1	2.20	0.41
2:H:78:GLN:HB3	2:H:80:ILE:HD11	2.03	0.41
2:H:30:SER:O	2:H:31:ASP:HB3	2.21	0.41
1:L:157:ASP:HA	1:L:197:SER:O	2.21	0.40
1:L:42:TYR:OH	1:L:95:GLN:NE2	2.49	0.40
1:L:156:ILE:O	1:L:198:TYR:HA	2.22	0.40
1:L:218:ASN:OD1	1:L:218:ASN:C	2.59	0.40
2:H:58:TYR:CE1	2:H:74:ARG:HD2	2.55	0.40
1:L:150:ILE:O	1:L:150:ILE:CG2	2.69	0.40
1:L:131:LEU:C	1:L:133:SER:H	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:4:MET:HE3	1:L:4:MET:HA	2.04	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:132:THR:OG1	2:H:19:ARG:NH2[4_665]	0.98	1.22
1:L:15:ALA:O	2:H:1:GLU:OE2[2_665]	1.41	0.79
1:L:132:THR:CB	2:H:19:ARG:NH2[4_665]	1.64	0.56
1:L:132:THR:CG2	2:H:19:ARG:NH2[4_665]	2.01	0.19
1:L:15:ALA:C	2:H:1:GLU:OE2[2_665]	2.06	0.14
1:L:132:THR:CG2	2:H:19:ARG:CZ[4_665]	2.09	0.11
1:L:18:ARG:NH2	2:H:108:TYR:OH[2_665]	2.17	0.03
1:L:132:THR:CG2	2:H:19:ARG:NH1[4_665]	2.17	0.03

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	L	218/220 (99%)	181 (83%)	30 (14%)	7 (3%)	4	22
2	H	220/222 (99%)	190 (86%)	19 (9%)	11 (5%)	2	13
All	All	438/442 (99%)	371 (85%)	49 (11%)	18 (4%)	3	16

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	218	ASN
2	H	30	SER
2	H	58	TYR
2	H	168	LYS
2	H	170	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	199	PRO
1	L	132	THR
1	L	156	ILE
1	L	161	ARG
1	L	217	ARG
2	H	57	LYS
2	H	203	SER
1	L	206	THR
2	H	142	ASP
1	L	193	GLU
2	H	137	PRO
2	H	180	ALA
2	H	48	ILE

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	L	195/195 (100%)	143 (73%)	52 (27%)	0	1
2	H	189/189 (100%)	142 (75%)	47 (25%)	0	2
All	All	384/384 (100%)	285 (74%)	99 (26%)	0	1

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	21	MET
1	L	23	CYS
1	L	24	LYS
1	L	27	GLN
1	L	30	LEU
1	L	36	LYS
1	L	37	ASN
1	L	38	PHE
1	L	45	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	52	LEU
1	L	53	LEU
1	L	60	ARG
1	L	71	SER
1	L	76	ASP
1	L	79	LEU
1	L	82	SER
1	L	87	GLU
1	L	95	GLN
1	L	96	ASN
1	L	102	LEU
1	L	110	LEU
1	L	111	GLU
1	L	113	LYS
1	L	122	SER
1	L	123	ILE
1	L	143	ASN
1	L	148	LYS
1	L	153	LYS
1	L	168	SER
1	L	170	THR
1	L	171	ASP
1	L	176	ASP
1	L	177	SER
1	L	178	THR
1	L	180	SER
1	L	181	MET
1	L	185	LEU
1	L	187	LEU
1	L	194	ARG
1	L	196	ASN
1	L	201	GLU
1	L	203	THR
1	L	206	THR
1	L	207	SER
1	L	208	THR
1	L	209	SER
1	L	213	LYS
1	L	214	SER
1	L	215	PHE
1	L	218	ASN
1	L	220	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	1	GLU
2	H	3	LYS
2	H	5	VAL
2	H	6	GLU
2	H	13	GLN
2	H	19	ARG
2	H	24	THR
2	H	38	ARG
2	H	46	GLU
2	H	51	SER
2	H	53	ASN
2	H	54	LYS
2	H	57	LYS
2	H	59	THR
2	H	63	SER
2	H	65	SER
2	H	71	ILE
2	H	74	ARG
2	H	89	ARG
2	H	91	GLU
2	H	105	SER
2	H	106	THR
2	H	110	ASP
2	H	117	THR
2	H	119	THR
2	H	122	SER
2	H	123	GLU
2	H	127	ASN
2	H	129	THR
2	H	134	THR
2	H	141	SER
2	H	144	VAL
2	H	146	ILE
2	H	156	SER
2	H	158	THR
2	H	166	SER
2	H	168	LYS
2	H	179	LEU
2	H	187	MET
2	H	188	SER
2	H	190	GLN
2	H	192	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	198	CYS
2	H	202	GLU
2	H	208	VAL
2	H	209	GLN
2	H	220	VAL

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

Mol	Chain	Res	Type
1	L	31	ASN
1	L	34	ASN
1	L	43	GLN
1	L	95	GLN
1	L	96	ASN
1	L	130	GLN
1	L	172	GLN
1	L	195	HIS
1	L	196	ASN
1	L	218	ASN
2	H	127	ASN
2	H	216	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	PC	H	223	-	10,10,10	0.94	0	15,15,15	1.44	2 (13%)

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
3	PC	H	223	-	-	5/8/8/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	H	223	PC	O4-P1-O3	3.86	122.38	107.64
3	H	223	PC	O2-P1-O1	-2.25	100.18	106.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	223	PC	C1-O2-P1-O1
3	H	223	PC	C1-O2-P1-O3
3	H	223	PC	C1-O2-P1-O4
3	H	223	PC	C2-C1-O2-P1
3	H	223	PC	O2-C1-C2-N1

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	223	PC	7	0

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](#)

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	L	71/220 (32%)	-0.89	4 (5%) 24 11	2, 4, 19, 43	0
2	H	174/222 (78%)	-1.07	0 100 100	2, 7, 17, 23	0
All	All	245/442 (55%)	-1.02	4 (1%) 72 51	2, 7, 18, 43	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	166	LEU	6.0
1	L	77	PHE	3.3
1	L	59	THR	3.1
1	L	220	CYS	2.1

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. 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	B-factors(Å ²)	Q<0.9
3	PC	H	223	11/11	0.84	0.41	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.