



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:08 PM UTC

PDB ID : 1PPP / pdb_00001ppp
Title : CRYSTAL STRUCTURE OF PAPAIN-E64-C COMPLEX. BINDING DIVERSITY OF E64-C TO PAPAIN S2 AND S3 SUBSITES
Authors : Ishida, T.
Deposited on : 1993-03-17
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

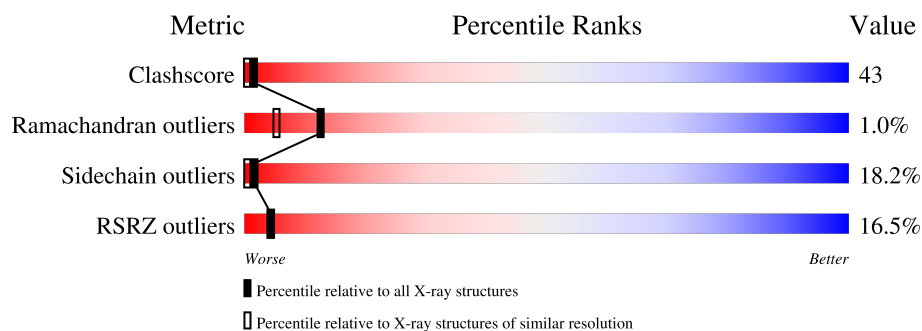
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	212	

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	E6C	A	213	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1884 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.

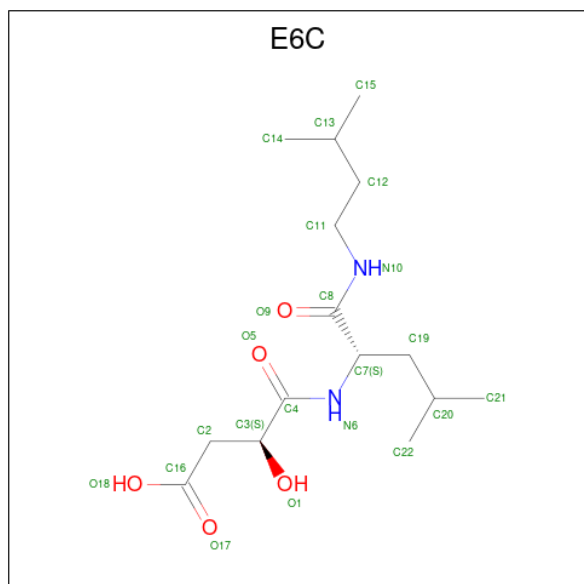
- Molecule 1 is a protein called PAPAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1655	1050	293	305	7			

There are 3 discrepancies between the modelled and reference sequences:

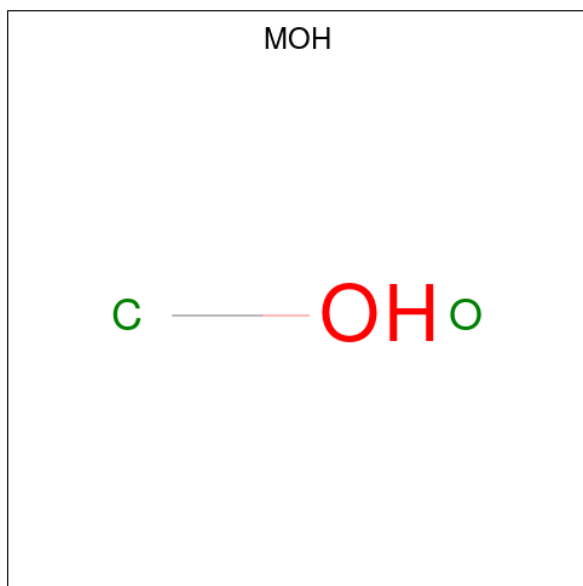
Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLN	GLU	conflict	UNP P00784
A	118	GLN	GLU	conflict	UNP P00784
A	135	GLN	GLU	conflict	UNP P00784

- Molecule 2 is N-[1-HYDROXYCARBOXYETHYL-CARBONYL]LEUCYLAMINO-2-METHYL-BUTANE (CCD ID: E6C) (formula: $C_{15}H_{28}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	15	2	5		

- Molecule 3 is METHANOL (CCD ID: MOH) (formula: CH₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			2	1	1		

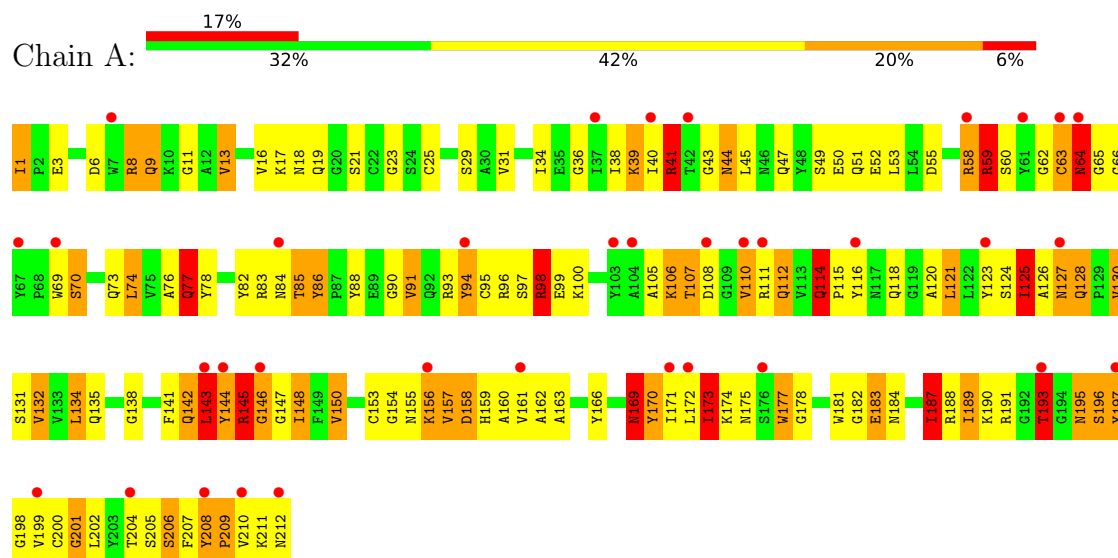
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	205	Total	O	0	0
			205	205		

3 Residue-property plots [i](#)

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: PAPAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.37Å 102.34Å 49.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90 200.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90) 66.4 (200.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.194 , (Not available) 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	9.8	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 360.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	1884	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.61% 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: E6C, MOH

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	1.05	1/1699 (0.1%)	2.48	132/2306 (5.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	3	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	GLY	N-CA	7.13	1.53	1.45

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	GLY	CA-C-O	-14.78	104.86	122.15
1	A	100	LYS	N-CA-C	12.64	127.09	112.93
1	A	208	TYR	O-C-N	11.99	130.24	121.85
1	A	74	LEU	CA-C-O	-10.74	109.03	120.42
1	A	64	ASN	CA-C-N	9.79	140.60	121.41
1	A	64	ASN	C-N-CA	9.79	140.60	121.41
1	A	146	GLY	N-CA-C	-9.33	99.33	111.37
1	A	108	ASP	CA-C-O	-9.17	109.46	120.55
1	A	197	TYR	O-C-N	9.15	132.58	122.15
1	A	147	GLY	N-CA-C	8.60	133.57	113.18
1	A	163	ALA	CA-C-O	-8.53	110.87	120.43
1	A	99	GLU	CA-CB-CG	8.46	131.03	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ARG	NE-CZ-NH2	-8.46	111.59	119.20
1	A	83	ARG	CD-NE-CZ	8.44	136.21	124.40
1	A	31	VAL	CA-C-O	-8.42	112.19	120.95
1	A	171	ILE	CA-C-O	-8.24	111.03	120.67
1	A	153	CYS	CA-C-N	8.19	130.37	122.27
1	A	153	CYS	C-N-CA	8.19	130.37	122.27
1	A	59	ARG	NE-CZ-NH2	8.08	126.47	119.20
1	A	44	ASN	OD1-CG-ND2	7.91	130.51	122.60
1	A	31	VAL	O-C-N	7.81	129.44	121.87
1	A	177	TRP	CA-C-N	-7.77	110.85	122.04
1	A	177	TRP	C-N-CA	-7.77	110.85	122.04
1	A	105	ALA	CA-C-O	7.76	129.43	120.89
1	A	59	ARG	CA-CB-CG	7.68	129.45	114.10
1	A	169	ASN	CA-C-O	-7.67	110.19	119.32
1	A	1	ILE	N-CA-CB	-7.67	98.46	111.50
1	A	169	ASN	CB-CG-ND2	7.65	127.88	116.40
1	A	198	GLY	CA-C-O	-7.64	116.10	122.29
1	A	65	GLY	N-CA-C	7.58	131.15	113.18
1	A	36	GLY	O-C-N	7.54	129.43	122.19
1	A	49	SER	N-CA-C	7.41	120.15	108.67
1	A	1	ILE	CB-CA-C	7.32	126.23	111.60
1	A	195	ASN	CB-CA-C	7.26	121.69	109.48
1	A	193	THR	CA-C-O	7.21	128.26	119.97
1	A	64	ASN	CA-CB-CG	7.04	119.64	112.60
1	A	126	ALA	O-C-N	6.98	130.85	122.27
1	A	91	VAL	CA-C-O	-6.97	112.86	120.67
1	A	123	TYR	N-CA-CB	6.96	120.10	110.01
1	A	59	ARG	CB-CA-C	6.90	124.15	110.42
1	A	209	PRO	CA-C-N	6.76	132.40	123.06
1	A	209	PRO	C-N-CA	6.76	132.40	123.06
1	A	123	TYR	CA-C-O	-6.70	113.78	120.82
1	A	205	SER	N-CA-CB	-6.57	99.39	110.49
1	A	132	VAL	N-CA-CB	-6.56	100.22	112.36
1	A	39	LYS	O-C-N	6.50	130.27	122.27
1	A	98	ARG	CD-NE-CZ	6.50	133.50	124.40
1	A	123	TYR	O-C-N	6.46	128.72	122.07
1	A	202	LEU	N-CA-C	6.45	120.00	111.75
1	A	195	ASN	N-CA-C	-6.44	99.20	109.76
1	A	114	GLN	O-C-N	6.41	126.89	121.31
1	A	84	ASN	CA-CB-CG	-6.41	106.19	112.60
1	A	9	GLN	OE1-CD-NE2	6.37	128.97	122.60
1	A	59	ARG	N-CA-CB	-6.35	99.76	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	NE-CZ-NH2	-6.34	113.49	119.20
1	A	142	GLN	O-C-N	6.29	128.79	122.12
1	A	64	ASN	CA-C-O	6.29	129.50	120.51
1	A	148	ILE	N-CA-CB	6.27	119.03	111.31
1	A	141	PHE	N-CA-CB	6.26	119.05	109.91
1	A	29	SER	O-C-N	6.25	128.51	122.07
1	A	124	SER	O-C-N	6.22	128.71	122.12
1	A	127	ASN	CA-CB-CG	-6.22	106.38	112.60
1	A	18	ASN	CA-C-O	6.14	126.86	120.30
1	A	112	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	A	91	VAL	CB-CA-C	6.11	119.90	110.50
1	A	69	TRP	O-C-N	6.07	128.55	122.12
1	A	128	GLN	CB-CG-CD	6.06	122.90	112.60
1	A	120	ALA	CA-C-O	-6.03	114.16	120.55
1	A	91	VAL	CA-CB-CG1	5.99	120.58	110.40
1	A	125	ILE	O-C-N	5.99	127.92	121.87
1	A	62	GLY	CA-C-O	-5.96	113.93	121.44
1	A	158	ASP	N-CA-CB	-5.96	99.22	111.07
1	A	43	GLY	N-CA-C	-5.94	107.49	115.21
1	A	59	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	A	147	GLY	O-C-N	-5.94	114.98	122.70
1	A	121	LEU	O-C-N	5.93	128.49	122.09
1	A	96	ARG	NH1-CZ-NH2	-5.92	111.61	119.30
1	A	158	ASP	CB-CG-OD1	5.91	131.99	118.40
1	A	82	TYR	N-CA-CB	5.89	118.70	110.04
1	A	143	LEU	CA-C-O	-5.80	111.69	119.11
1	A	177	TRP	O-C-N	-5.80	115.12	122.43
1	A	184	ASN	N-CA-C	-5.80	104.82	112.24
1	A	198	GLY	N-CA-C	-5.68	105.52	112.68
1	A	193	THR	N-CA-C	-5.66	105.26	111.82
1	A	83	ARG	NE-CZ-NH1	5.63	127.13	121.50
1	A	43	GLY	CA-C-O	-5.63	112.97	119.10
1	A	63	CYS	CA-C-O	-5.62	114.86	121.16
1	A	170	TYR	CA-C-O	-5.62	115.40	121.36
1	A	86	TYR	CB-CA-C	5.56	119.44	111.27
1	A	96	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	A	142	GLN	CA-CB-CG	-5.54	103.01	114.10
1	A	175	ASN	CA-C-O	-5.53	115.42	121.89
1	A	38	ILE	CA-C-O	-5.52	115.21	120.95
1	A	160	ALA	CA-C-O	-5.51	114.58	120.92
1	A	206	SER	N-CA-CB	-5.51	101.25	110.83
1	A	183	GLU	CG-CD-OE1	5.50	131.05	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	TYR	CA-C-O	-5.46	115.14	121.15
1	A	126	ALA	CA-C-O	-5.44	113.71	119.97
1	A	196	SER	O-C-N	5.44	128.96	122.27
1	A	70	SER	CA-C-O	5.42	126.51	120.82
1	A	197	TYR	CA-C-O	-5.40	114.70	120.42
1	A	160	ALA	O-C-N	5.37	129.38	123.16
1	A	100	LYS	CA-CB-CG	-5.34	103.42	114.10
1	A	177	TRP	CA-C-O	-5.32	114.97	121.88
1	A	114	GLN	CA-C-O	-5.29	114.33	119.51
1	A	208	TYR	N-CA-CB	5.28	120.15	111.17
1	A	82	TYR	O-C-N	5.27	129.29	122.81
1	A	23	GLY	CA-C-N	5.25	131.02	122.67
1	A	23	GLY	C-N-CA	5.25	131.02	122.67
1	A	193	THR	N-CA-CB	-5.25	102.14	110.28
1	A	8	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	A	84	ASN	CB-CG-ND2	-5.22	108.57	116.40
1	A	169	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	83	ARG	CA-C-O	-5.19	114.00	119.97
1	A	173	ILE	CB-CA-C	-5.19	102.51	110.50
1	A	201	GLY	CA-C-N	5.18	127.94	120.38
1	A	201	GLY	C-N-CA	5.18	127.94	120.38
1	A	53	LEU	N-CA-C	-5.17	105.55	111.14
1	A	172	LEU	CA-C-O	-5.17	114.70	120.54
1	A	157	VAL	O-C-N	5.16	128.10	122.63
1	A	126	ALA	N-CA-CB	5.15	118.27	110.28
1	A	41	ARG	N-CA-C	5.15	117.68	111.40
1	A	169	ASN	CB-CG-OD1	-5.14	110.52	120.80
1	A	74	LEU	O-C-N	5.14	128.01	122.15
1	A	64	ASN	O-C-N	-5.12	115.78	122.59
1	A	77	GLN	N-CA-C	5.12	116.55	110.97
1	A	11	GLY	O-C-N	5.03	129.24	122.70
1	A	108	ASP	CB-CA-C	-5.03	103.03	111.13
1	A	187	ILE	O-C-N	-5.02	117.65	123.07
1	A	50	GLU	O-C-N	5.02	127.87	122.15
1	A	97	SER	O-C-N	5.01	127.87	122.11
1	A	47	GLN	CA-CB-CG	-5.00	104.09	114.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	ILE	CB
1	A	125	ILE	CB

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Mol	Chain	Res	Type	Atom
1	A	173	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Sidechain

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	1655	0	1595	136	1
2	A	22	0	25	17	0
3	A	2	0	0	1	0
4	A	205	0	0	19	3
All	All	1884	0	1620	141	3

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 43.

All (141) 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:A:173:ILE:CG2	1:A:187:ILE:HG22	1.64	1.27
1:A:173:ILE:CG2	1:A:187:ILE:CG2	2.22	1.16
1:A:173:ILE:HG23	1:A:187:ILE:CG2	1.76	1.14
1:A:41:ARG:HD2	1:A:41:ARG:N	1.38	1.10
1:A:193:THR:HB	4:A:391:HOH:O	1.60	1.02
1:A:116:TYR:HB3	1:A:196:SER:OG	1.61	1.01
1:A:150:VAL:HG23	4:A:383:HOH:O	1.59	1.00
1:A:98:ARG:HG3	1:A:98:ARG:HH11	1.24	0.98
1:A:173:ILE:HG23	1:A:187:ILE:HG22	0.99	0.97
1:A:107:THR:HG21	4:A:230:HOH:O	1.66	0.95
1:A:85:THR:HG21	4:A:339:HOH:O	1.66	0.94
1:A:116:TYR:HB3	1:A:196:SER:HG	1.30	0.93
1:A:156:LYS:HE3	4:A:387:HOH:O	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:N	1:A:41:ARG:CD	2.32	0.91
1:A:161:VAL:HG13	1:A:174:LYS:O	1.74	0.88
1:A:66:GLY:O	2:A:213:E6C:H20	1.75	0.86
1:A:173:ILE:CG2	1:A:187:ILE:HG23	2.05	0.86
1:A:106:LYS:O	1:A:211:LYS:NZ	2.07	0.86
1:A:156:LYS:HD2	4:A:387:HOH:O	1.76	0.86
1:A:173:ILE:HG21	1:A:187:ILE:CG2	2.04	0.85
1:A:64:ASN:C	1:A:64:ASN:HD22	1.84	0.83
1:A:158:ASP:HA	2:A:213:E6C:H121	1.60	0.83
1:A:25:CYS:HB3	2:A:213:E6C:O17	1.80	0.82
1:A:135:GLN:HE21	1:A:156:LYS:HG3	1.44	0.82
1:A:193:THR:CG2	1:A:195:ASN:HB3	2.11	0.81
1:A:94:TYR:H	1:A:94:TYR:HD1	1.26	0.81
1:A:118:GLN:NE2	1:A:191:ARG:HH11	1.79	0.79
1:A:3:GLU:HG2	4:A:253:HOH:O	1.83	0.78
1:A:193:THR:CG2	4:A:247:HOH:O	2.32	0.77
1:A:193:THR:HG22	1:A:195:ASN:HB3	1.67	0.76
1:A:157:VAL:O	2:A:213:E6C:H153	1.86	0.76
1:A:40:ILE:C	1:A:41:ARG:HD2	2.10	0.75
1:A:211:LYS:HG3	1:A:212:ASN:H	1.51	0.75
1:A:144:TYR:CE2	1:A:187:ILE:HG12	2.24	0.72
1:A:125:ILE:CG2	1:A:166:TYR:HD2	2.03	0.71
1:A:199:VAL:HG13	4:A:384:HOH:O	1.88	0.71
1:A:193:THR:HG23	4:A:247:HOH:O	1.91	0.71
1:A:156:LYS:CD	4:A:387:HOH:O	2.34	0.69
1:A:146:GLY:HA2	1:A:183:GLU:HG2	1.76	0.68
1:A:144:TYR:CD2	1:A:187:ILE:HG12	2.29	0.67
1:A:60:SER:HB3	1:A:66:GLY:HA3	1.77	0.66
1:A:193:THR:HG22	1:A:195:ASN:H	1.61	0.66
1:A:59:ARG:NH1	1:A:73:GLN:NE2	2.44	0.66
2:A:213:E6C:H212	2:A:213:E6C:O9	1.96	0.65
1:A:135:GLN:NE2	1:A:156:LYS:HG3	2.12	0.64
1:A:85:THR:CG2	4:A:339:HOH:O	2.37	0.62
1:A:59:ARG:HH12	1:A:73:GLN:NE2	1.96	0.62
1:A:118:GLN:HE21	1:A:191:ARG:HH11	1.45	0.61
1:A:187:ILE:HD13	1:A:188:ARG:N	2.15	0.61
1:A:39:LYS:HG3	1:A:45:LEU:HB2	1.83	0.61
1:A:169:ASN:H	1:A:169:ASN:HD22	1.47	0.61
1:A:193:THR:HG21	4:A:247:HOH:O	1.96	0.61
1:A:146:GLY:HA2	1:A:183:GLU:CG	2.31	0.60
1:A:98:ARG:HG3	1:A:98:ARG:NH1	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:HE21	1:A:191:ARG:NH1	2.00	0.60
1:A:58:ARG:HD2	4:A:418:HOH:O	2.01	0.60
1:A:41:ARG:HD2	1:A:41:ARG:H	1.58	0.59
1:A:66:GLY:O	2:A:213:E6C:C20	2.50	0.59
1:A:155:ASN:ND2	1:A:197:TYR:CD2	2.71	0.59
1:A:173:ILE:HD13	1:A:189:ILE:HG13	1.84	0.58
1:A:135:GLN:HE21	1:A:156:LYS:CG	2.16	0.57
1:A:74:LEU:CD2	1:A:78:TYR:CD2	2.87	0.56
1:A:161:VAL:CG1	1:A:162:ALA:H	2.19	0.56
1:A:211:LYS:HG3	1:A:212:ASN:N	2.17	0.56
1:A:64:ASN:O	1:A:64:ASN:ND2	2.37	0.56
1:A:161:VAL:HG12	1:A:162:ALA:N	2.21	0.55
1:A:66:GLY:H	2:A:213:E6C:H222	1.72	0.55
1:A:8:ARG:HA	1:A:13:VAL:HG13	1.89	0.55
1:A:118:GLN:NE2	1:A:191:ARG:NH1	2.53	0.55
1:A:193:THR:HG22	1:A:195:ASN:N	2.22	0.54
1:A:125:ILE:CG2	1:A:166:TYR:CD2	2.88	0.54
1:A:128:GLN:NE2	1:A:208:TYR:HB2	2.22	0.54
1:A:39:LYS:HA	1:A:44:ASN:O	2.08	0.54
2:A:213:E6C:C8	2:A:213:E6C:H223	2.37	0.54
1:A:211:LYS:CG	1:A:212:ASN:N	2.71	0.53
1:A:74:LEU:HD22	1:A:78:TYR:CD2	2.44	0.53
1:A:41:ARG:CG	1:A:41:ARG:HH11	2.22	0.53
1:A:114:GLN:HE21	1:A:115:PRO:HD2	1.73	0.53
1:A:131:SER:O	1:A:206:SER:HA	2.09	0.52
1:A:170:TYR:OH	3:A:214:MOH:C	2.57	0.52
1:A:76:ALA:HA	1:A:107:THR:O	2.10	0.52
1:A:161:VAL:CG1	1:A:162:ALA:N	2.72	0.52
1:A:25:CYS:CB	2:A:213:E6C:O17	2.56	0.52
1:A:156:LYS:CE	4:A:387:HOH:O	2.34	0.52
1:A:125:ILE:HG21	1:A:166:TYR:HD2	1.74	0.51
1:A:148:ILE:HD13	1:A:169:ASN:OD1	2.10	0.51
1:A:201:GLY:O	1:A:204:THR:OG1	2.19	0.51
2:A:213:E6C:O9	2:A:213:E6C:H223	2.11	0.51
1:A:135:GLN:HE22	1:A:154:GLY:HA3	1.76	0.50
1:A:66:GLY:N	2:A:213:E6C:C22	2.74	0.50
1:A:74:LEU:CD2	1:A:78:TYR:HD2	2.25	0.50
1:A:6:ASP:HB3	1:A:9:GLN:HG3	1.94	0.49
1:A:161:VAL:HG12	1:A:162:ALA:H	1.77	0.49
1:A:51:GLN:HB2	1:A:88:TYR:HA	1.95	0.49
1:A:52:GLU:HG3	1:A:86:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:HG2	1:A:70:SER:OG	2.12	0.49
1:A:74:LEU:HD22	1:A:78:TYR:HD2	1.78	0.49
1:A:40:ILE:HG22	1:A:41:ARG:NE	2.28	0.49
1:A:130:VAL:HG22	1:A:208:TYR:HB3	1.95	0.49
1:A:111:ARG:HG3	1:A:210:VAL:CG2	2.44	0.48
1:A:59:ARG:NH1	1:A:73:GLN:HE22	2.13	0.47
1:A:127:ASN:O	1:A:128:GLN:HB3	2.15	0.47
1:A:73:GLN:O	1:A:77:GLN:HG2	2.15	0.46
1:A:19:GLN:NE2	2:A:213:E6C:O17	2.46	0.46
1:A:40:ILE:HG22	1:A:41:ARG:HE	1.81	0.46
1:A:58:ARG:HB3	4:A:321:HOH:O	2.16	0.46
1:A:110:VAL:HG22	4:A:230:HOH:O	2.16	0.46
1:A:135:GLN:NE2	1:A:156:LYS:CG	2.77	0.46
1:A:66:GLY:N	2:A:213:E6C:H222	2.30	0.46
1:A:64:ASN:C	1:A:64:ASN:ND2	2.63	0.45
1:A:121:LEU:HG	1:A:125:ILE:HD11	1.99	0.45
1:A:41:ARG:NH1	1:A:41:ARG:HG3	2.32	0.44
1:A:159:HIS:HA	2:A:213:E6C:H22	1.99	0.44
1:A:41:ARG:CG	1:A:41:ARG:NH1	2.80	0.44
1:A:112:GLN:HB2	1:A:207:PHE:CE2	2.51	0.44
1:A:138:GLY:O	1:A:142:GLN:HG3	2.16	0.44
2:A:213:E6C:H191	2:A:213:E6C:H122	1.99	0.44
1:A:88:TYR:CZ	1:A:90:GLY:HA2	2.52	0.44
1:A:145:ARG:HA	1:A:182:GLY:HA2	2.00	0.44
1:A:169:ASN:H	1:A:169:ASN:ND2	2.16	0.44
1:A:17:LYS:O	1:A:177:TRP:O	2.36	0.43
2:A:213:E6C:H222	2:A:213:E6C:O5	2.19	0.43
1:A:74:LEU:CD2	1:A:78:TYR:CE2	3.02	0.43
1:A:94:TYR:CD1	1:A:94:TYR:N	2.74	0.43
1:A:121:LEU:O	1:A:125:ILE:HG13	2.19	0.42
1:A:143:LEU:HA	1:A:143:LEU:HD13	1.13	0.42
1:A:55:ASP:O	1:A:95:CYS:HB2	2.20	0.42
1:A:181:TRP:CH2	1:A:187:ILE:HB	2.55	0.42
1:A:66:GLY:N	2:A:213:E6C:H221	2.33	0.42
1:A:154:GLY:O	1:A:200:CYS:HA	2.20	0.42
1:A:208:TYR:HB2	1:A:209:PRO:HD2	2.01	0.42
1:A:63:CYS:O	1:A:64:ASN:ND2	2.53	0.41
1:A:77:GLN:HG2	1:A:77:GLN:H	1.55	0.41
1:A:187:ILE:HD12	1:A:189:ILE:HG12	2.02	0.41
1:A:134:LEU:C	1:A:134:LEU:HD12	2.46	0.41
1:A:148:ILE:CD1	1:A:169:ASN:OD1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:CD1	1:A:166:TYR:C	2.98	0.41
1:A:17:LYS:HB3	4:A:275:HOH:O	2.20	0.41
1:A:39:LYS:HG2	1:A:44:ASN:C	2.45	0.41
1:A:9:GLN:NE2	4:A:257:HOH:O	2.29	0.41
1:A:193:THR:HG21	1:A:195:ASN:HB3	1.98	0.40

All (3) 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)
4:A:242:HOH:O	4:A:307:HOH:O[1_655]	1.69	0.51
1:A:94:TYR:OH	4:A:275:HOH:O[4_456]	1.78	0.42
4:A:253:HOH:O	4:A:370:HOH:O[2_865]	1.94	0.26

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	210/212 (99%)	197 (94%)	11 (5%)	2 (1%)	12 5

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	64	ASN

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	170/170 (100%)	139 (82%)	31 (18%)	2 0

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	13	VAL
1	A	16	VAL
1	A	21	SER
1	A	34	ILE
1	A	41	ARG
1	A	58	ARG
1	A	64	ASN
1	A	77	GLN
1	A	85	THR
1	A	91	VAL
1	A	94	TYR
1	A	98	ARG
1	A	106	LYS
1	A	107	THR
1	A	110	VAL
1	A	114	GLN
1	A	125	ILE
1	A	130	VAL
1	A	132	VAL
1	A	134	LEU
1	A	143	LEU
1	A	145	ARG
1	A	150	VAL
1	A	156	LYS
1	A	169	ASN
1	A	173	ILE
1	A	187	ILE
1	A	189	ILE
1	A	190	LYS
1	A	193	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	73	GLN
1	A	77	GLN
1	A	84	ASN
1	A	114	GLN
1	A	127	ASN
1	A	135	GLN
1	A	184	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	MOH	A	214	-	1,1,1	0.65	0	-		
2	E6C	A	213	1	21,21,21	1.26	2 (9%)	25,27,27	1.93	5 (20%)

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	E6C	A	213	1	-	10/26/26/26	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	213	E6C	O18-C16	-3.02	1.20	1.30
2	A	213	E6C	C7-N6	-2.89	1.39	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	213	E6C	C19-C7-N6	5.37	122.69	110.58
2	A	213	E6C	C20-C19-C7	-3.44	106.16	115.40
2	A	213	E6C	C19-C7-C8	3.07	117.86	110.59
2	A	213	E6C	C12-C11-N10	-2.59	104.77	111.88
2	A	213	E6C	O17-C16-C2	-2.02	116.63	122.84

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	213	E6C	C7-C8-N10-C11
2	A	213	E6C	O9-C8-N10-C11
2	A	213	E6C	C12-C11-N10-C8
2	A	213	E6C	C20-C19-C7-N6
2	A	213	E6C	C7-C19-C20-C22
2	A	213	E6C	C7-C19-C20-C21
2	A	213	E6C	C19-C7-N6-C4
2	A	213	E6C	O1-C3-C4-O5
2	A	213	E6C	C20-C19-C7-C8
2	A	213	E6C	N10-C11-C12-C13

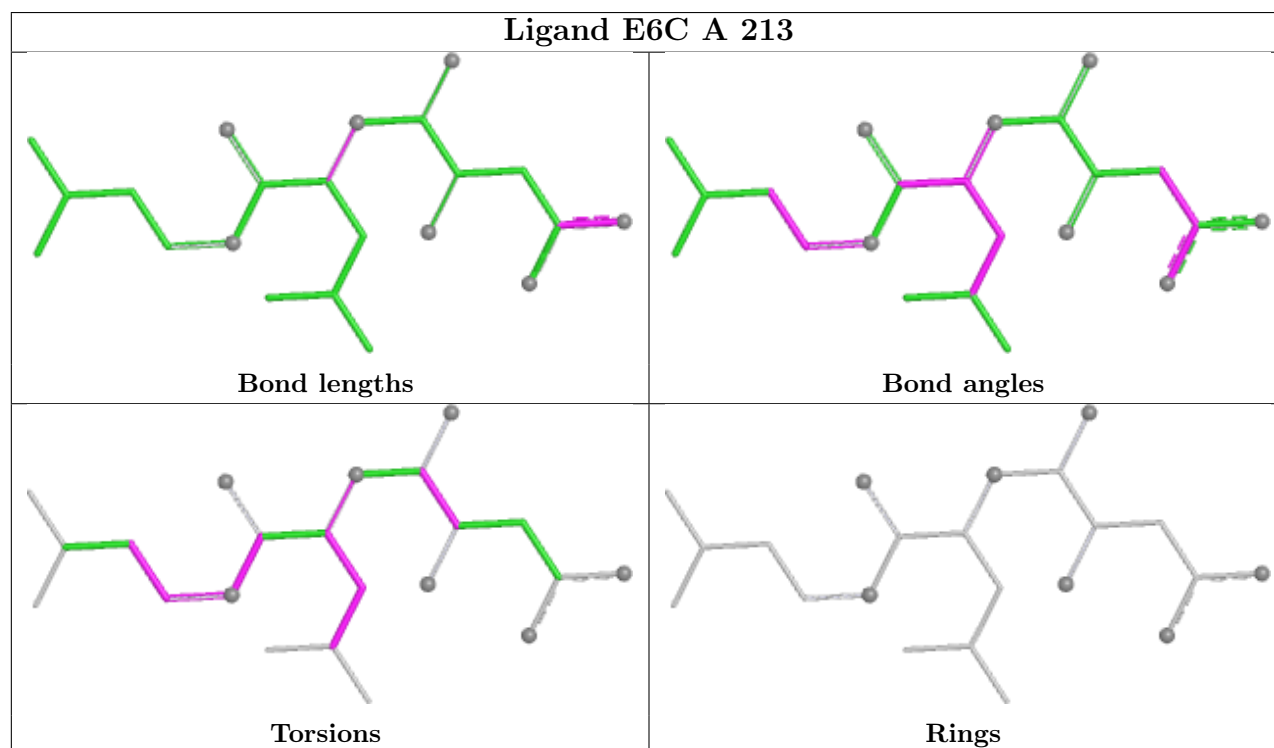
There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	214	MOH	1	0
2	A	213	E6C	17	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	212/212 (100%)	1.05	35 (16%) 4 4	3, 10, 23, 37	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	TYR	4.0
1	A	204	THR	3.6
1	A	197	TYR	3.6
1	A	212	ASN	3.5
1	A	208	TYR	3.5
1	A	143	LEU	3.4
1	A	144	TYR	3.3
1	A	123	TYR	3.3
1	A	103	TYR	3.0
1	A	111	ARG	3.0
1	A	58	ARG	2.9
1	A	63	CYS	2.9
1	A	84	ASN	2.8
1	A	199	VAL	2.8
1	A	146	GLY	2.8
1	A	69	TRP	2.8
1	A	210	VAL	2.8
1	A	104	ALA	2.6
1	A	64	ASN	2.6
1	A	172	LEU	2.5
1	A	193	THR	2.5
1	A	156	LYS	2.5
1	A	37	ILE	2.4
1	A	7	TRP	2.3
1	A	61	TYR	2.3
1	A	161	VAL	2.3
1	A	42	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	67	TYR	2.2
1	A	108	ASP	2.2
1	A	116	TYR	2.2
1	A	40	ILE	2.1
1	A	127	ASN	2.1
1	A	176	SER	2.1
1	A	110	VAL	2.1
1	A	171	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

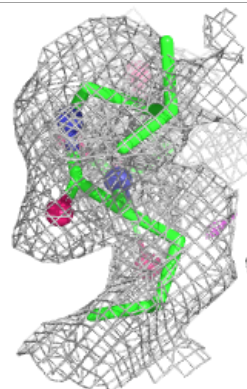
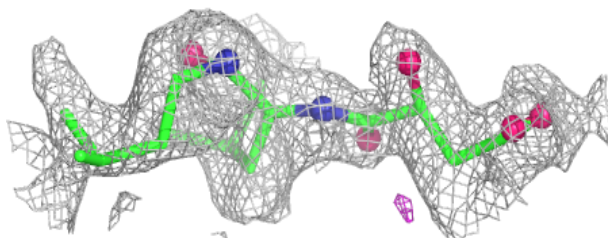
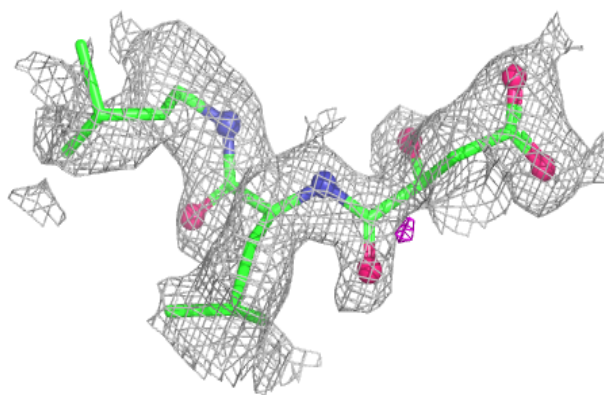
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	E6C	A	213	22/22	0.80	0.14	20,26,26,27	0
3	MOH	A	214	2/2	0.94	0.12	28,28,28,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around E6C A 213:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.