



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:34 PM GMT

PDB ID : 1PPP  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

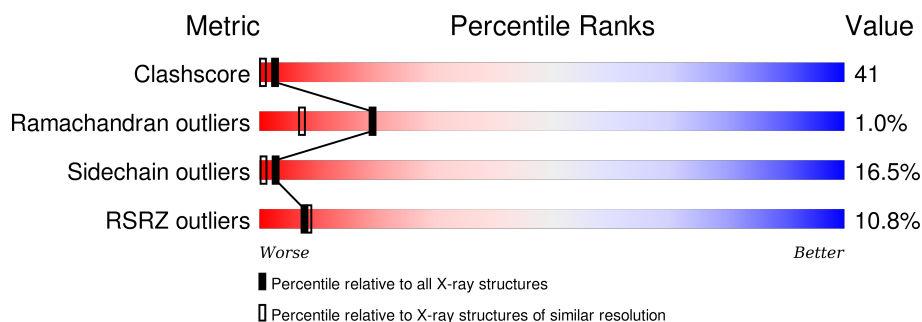
# 1 Overall quality at a glance

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	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.

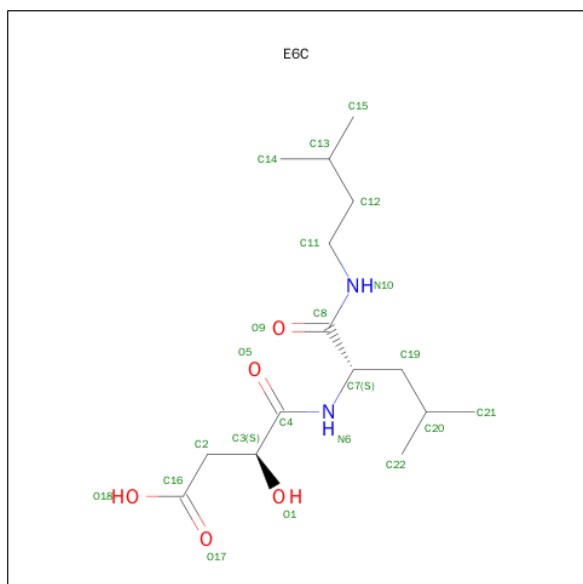
- Molecule 1 is a protein called PAPAIN.

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:

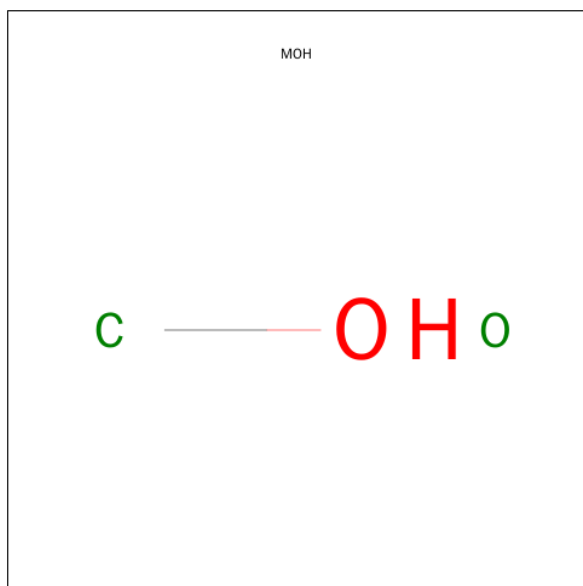
Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLN	GLU	CONFLICT	UNP P00784
A	118	GLN	GLU	CONFLICT	UNP P00784
A	135	GLN	GLU	CONFLICT	UNP P00784

- Molecule 2 is N-[1-HYDROXYCARBOXYETHYL-CARBONYL]LEUCYLAMINO-2-METHYL-BUTANE (three-letter code: E6C) (formula: C<sub>15</sub>H<sub>28</sub>N<sub>2</sub>O<sub>5</sub>).



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

- Molecule 3 is METHANOL (three-letter code: MOH) (formula: CH<sub>4</sub>O).



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

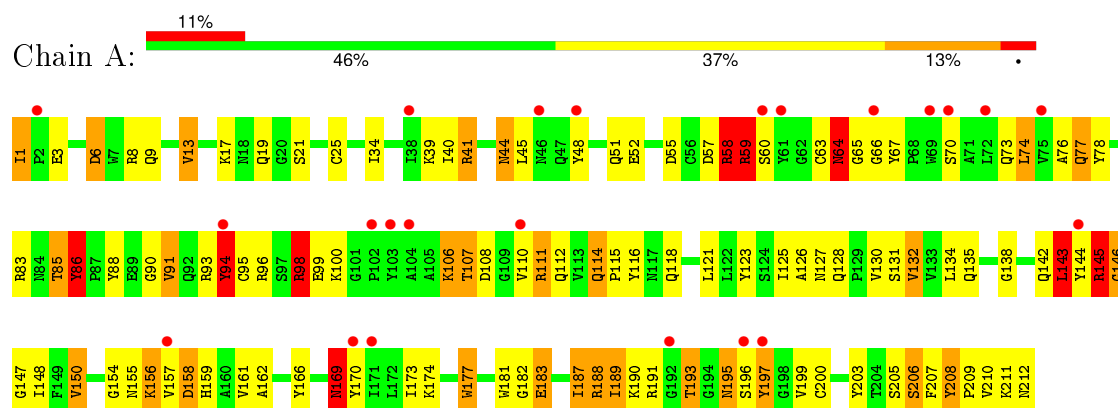
- Molecule 4 is water.

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	43.37Å 102.34Å 49.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90 51.17 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90) 66.4 (51.17-1.90)	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) (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	9.8	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 833.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 14810 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	1884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.81	0/1699	2.08	66/2306 (2.9%)

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

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ARG	NE-CZ-NH2	-17.43	111.59	120.30
1	A	158	ASP	CB-CG-OD1	15.21	131.99	118.30
1	A	83	ARG	NE-CZ-NH1	13.66	127.13	120.30
1	A	93	ARG	NE-CZ-NH2	-13.62	113.49	120.30
1	A	59	ARG	NE-CZ-NH2	12.34	126.47	120.30
1	A	93	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	A	67	TYR	CB-CG-CD2	10.29	127.17	121.00
1	A	67	TYR	CB-CG-CD1	-9.50	115.30	121.00
1	A	59	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	A	208	TYR	CB-CG-CD1	-9.27	115.44	121.00
1	A	83	ARG	CD-NE-CZ	9.01	136.21	123.60
1	A	146	GLY	CA-C-O	-8.74	104.86	120.60
1	A	64	ASN	C-N-CA	8.72	140.60	122.30
1	A	158	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	A	146	GLY	CA-C-N	8.29	132.79	116.20
1	A	147	GLY	N-CA-C	8.19	133.57	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	TYR	CB-CG-CD2	8.02	125.81	121.00
1	A	99	GLU	CA-CB-CG	8.01	131.03	113.40
1	A	208	TYR	CB-CG-CD2	7.83	125.70	121.00
1	A	96	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	96	ARG	NE-CZ-NH2	7.78	124.19	120.30
1	A	203	TYR	CB-CG-CD2	-7.58	116.45	121.00
1	A	183	GLU	OE1-CD-OE2	-7.46	114.35	123.30
1	A	205	SER	N-CA-CB	-7.40	99.39	110.50
1	A	1	ILE	CB-CA-C	7.32	126.23	111.60
1	A	59	ARG	CA-CB-CG	7.30	129.45	113.40
1	A	65	GLY	N-CA-C	7.22	131.15	113.10
1	A	96	ARG	NH1-CZ-NH2	-7.08	111.61	119.40
1	A	98	ARG	CD-NE-CZ	7.07	133.50	123.60
1	A	59	ARG	CB-CA-C	6.87	124.15	110.40
1	A	177	TRP	CA-C-N	6.81	129.82	116.20
1	A	188	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	203	TYR	CB-CG-CD1	6.68	125.01	121.00
1	A	48	TYR	CB-CG-CD1	6.54	124.92	121.00
1	A	91	VAL	CA-CB-CG1	6.45	120.58	110.90
1	A	183	GLU	CG-CD-OE1	6.38	131.05	118.30
1	A	86	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	A	158	ASP	N-CA-CB	-6.32	99.22	110.60
1	A	206	SER	N-CA-CB	-6.17	101.25	110.50
1	A	6	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	59	ARG	N-CA-CB	-6.02	99.76	110.60
1	A	100	LYS	N-CA-C	5.96	127.09	111.00
1	A	126	ALA	N-CA-CB	5.83	118.27	110.10
1	A	143	LEU	CA-CB-CG	-5.72	102.14	115.30
1	A	58	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	195	ASN	CB-CA-C	5.64	121.69	110.40
1	A	177	TRP	CB-CA-C	5.60	121.60	110.40
1	A	108	ASP	CA-C-N	5.59	127.38	116.20
1	A	169	ASN	CB-CG-OD1	-5.54	110.52	121.60
1	A	197	TYR	O-C-N	5.52	132.58	123.20
1	A	146	GLY	N-CA-C	-5.51	99.33	113.10
1	A	177	TRP	C-N-CA	-5.45	110.85	122.30
1	A	169	ASN	CA-C-N	5.40	129.08	117.20
1	A	1	ILE	N-CA-CB	-5.36	98.46	110.80
1	A	94	TYR	CB-CG-CD1	5.32	124.19	121.00
1	A	208	TYR	N-CA-CB	5.30	120.15	110.60
1	A	57	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	111	ARG	NE-CZ-NH1	-5.29	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	TYR	N-CA-CB	5.28	120.10	110.60
1	A	74	LEU	CA-C-O	-5.27	109.03	120.10
1	A	58	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	98	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	132	VAL	N-CA-CB	-5.13	100.22	111.50
1	A	126	ALA	O-C-N	5.09	130.85	122.70
1	A	108	ASP	CA-C-O	-5.07	109.46	120.10
1	A	59	ARG	CG-CD-NE	5.00	122.31	111.80

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	ILE	CB
1	A	125	ILE	CB
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	130	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	135	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 41.

All (135) 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:N	1:A:41:ARG:HD2	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:156:LYS:HE3	4:A:387:HOH:O	1.70	0.91
1:A:41:ARG:CD	1:A:41:ARG:N	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:158:ASP:HA	2:A:213:E6C:H121	1.60	0.83
1:A:135:GLN:HE21	1:A:156:LYS:HG3	1.44	0.82
1:A:25:CYS:HB3	2:A:213:E6C:O17	1.80	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:64:ASN:HD22	1:A:64:ASN:C	1.84	0.78
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: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:40:ILE:C	1:A:41:ARG:HD2	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:A:169:ASN:H	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:NH1	1:A:98:ARG:HG3	1.98	0.60
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:H	1:A:41:ARG:HD2	1.58	0.59
1:A:211:LYS:HG3	1:A:212:ASN:N	2.17	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: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:118:GLN:NE2	1:A:191:ARG:NH1	2.53	0.55
1:A:8:ARG:HA	1:A:13:VAL:HG13	1.89	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
2:A:213:E6C:C8	2:A:213:E6C:H223	2.37	0.54
1:A:39:LYS:HA	1:A:44:ASN:O	2.08	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:161:VAL:CG1	1:A:162:ALA:N	2.72	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:213:E6C:H223	2:A:213:E6C:O9	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:59:ARG:HG2	1:A:70:SER:OG	2.12	0.49
1:A:52:GLU:HG3	1:A:86:TYR:CE2	2.47	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:110:VAL:HG22	4:A:230:HOH:O	2.16	0.46
1:A:58:ARG:HB3	4:A:321: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: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:NH1	1:A:41:ARG:CG	2.80	0.44
1:A:112:GLN:HB2	1:A:207:PHE:CE2	2.51	0.44
2:A:213:E6C:H191	2:A:213:E6C:H122	1.99	0.44
1:A:138:GLY:O	1:A:142:GLN:HG3	2.16	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:94:TYR:CD1	1:A:94:TYR:N	2.74	0.43
1:A:74:LEU:CD2	1:A:78:TYR:CE2	3.02	0.43
1:A:121:LEU:O	1:A:125:ILE:HG13	2.19	0.42
1:A:143:LEU:HD13	1:A:143:LEU:HA	1.13	0.42
1:A:181:TRP:CH2	1:A:187:ILE:HB	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:O	1:A:95:CYS:HB2	2.20	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:187:ILE:HD12	1:A:189:ILE:HG12	2.02	0.41
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:148:ILE:CD1	1:A:169:ASN:OD1	2.69	0.41
1:A:17:LYS:HB3	4:A:275:HOH:O	2.20	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 [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	210/212 (99%)	197 (94%)	11 (5%)	2 (1%)	<b>19</b> <b>7</b>

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%)	142 (84%)	28 (16%)	<b>3</b> <b>1</b>

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	13	VAL
1	A	21	SER
1	A	34	ILE
1	A	41	ARG
1	A	44	ASN
1	A	58	ARG
1	A	64	ASN
1	A	77	GLN
1	A	85	THR
1	A	86	TYR
1	A	91	VAL
1	A	94	TYR
1	A	98	ARG
1	A	106	LYS
1	A	107	THR
1	A	114	GLN
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	187	ILE
1	A	189	ILE
1	A	190	LYS
1	A	193	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	128	GLN
1	A	135	GLN
1	A	142	GLN
1	A	155	ASN
1	A	169	ASN
1	A	184	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
2	E6C	A	213	1	17,21,21	1.01	1 (5%)	20,27,27	2.10	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MOH	A	214	-	1,1,1	0.57	0	0,0,0	0.00	-

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	-	0/24/26/26	0/0/0/0
3	MOH	A	214	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	213	E6C	C7-N6	-2.67	1.39	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	213	E6C	C20-C19-C7	-3.16	106.16	115.50
2	A	213	E6C	C3-C4-N6	-3.02	110.55	116.15
2	A	213	E6C	C19-C7-C8	2.79	117.86	110.60
2	A	213	E6C	C2-C3-C4	3.55	118.29	111.31
2	A	213	E6C	C19-C7-N6	4.89	122.69	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	212/212 (100%)	0.85	23 (10%) 8 8	3, 10, 23, 37	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	SER	4.6
1	A	38	ILE	4.2
1	A	48	TYR	3.4
1	A	144	TYR	3.4
1	A	75	VAL	3.3
1	A	157	VAL	3.1
1	A	192	GLY	3.1
1	A	2	PRO	3.0
1	A	94	TYR	2.9
1	A	72	LEU	2.9
1	A	66	GLY	2.8
1	A	103	TYR	2.6
1	A	60	SER	2.5
1	A	102	PRO	2.5
1	A	69	TRP	2.5
1	A	61	TYR	2.4
1	A	197	TYR	2.4
1	A	171	ILE	2.4
1	A	70	SER	2.4
1	A	170	TYR	2.3
1	A	104	ALA	2.3
1	A	110	VAL	2.3
1	A	46	ASN	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	MOH	A	214	2/2	0.95	0.14	0.11	28,28,28,29	0
2	E6C	A	213	22/22	0.83	0.17	0.11	20,26,26,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.