



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 09:29 pm GMT

PDB ID : 3GCH  
Title : CHEMISTRY OF CAGED ENZYMES. BINDING OF PHOTOREVERSIBLE CINNAMATES TO CHYMOTRYPSIN  
Authors : Stoddard, B.L.; Ringe, D.; Petsko, G.A.  
Deposited on : 1989-09-25  
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.

---

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

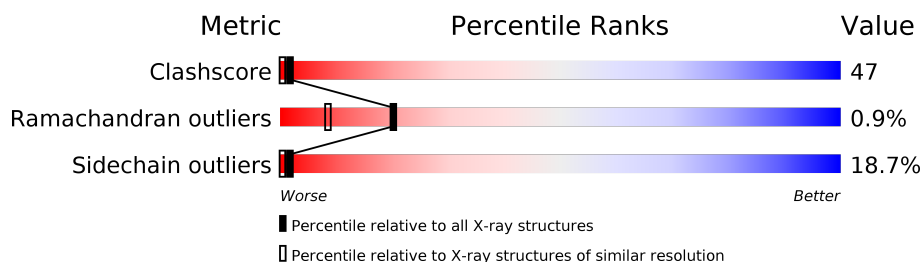
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

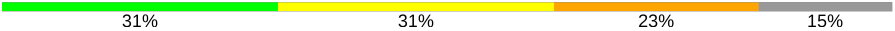
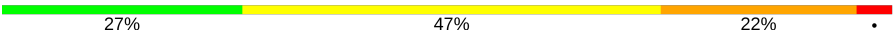
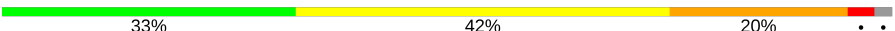
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	13	
2	B	131	
3	C	97	

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
4	OAC	C	246	X	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1824 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 GAMMA-CHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	11	Total	C	N	O	S	0	0	1
			69	45	12	11	1			

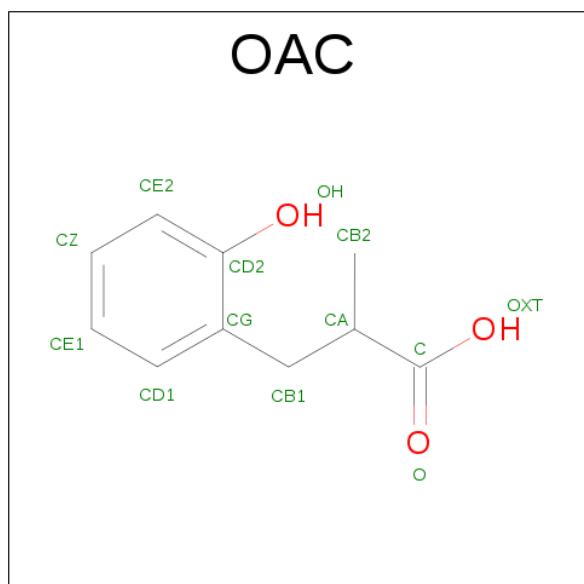
- Molecule 2 is a protein called GAMMA-CHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			979	618	162	195	4			

- Molecule 3 is a protein called GAMMA-CHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	95	Total	C	N	O	S	0	0	0
			688	429	120	132	7			

- Molecule 4 is TRANS-O-HYDROXY-ALPHA-METHYL CINNAMATE (three-letter code: OAC) (formula: C<sub>10</sub>H<sub>12</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			12	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	52	Total	O	0	0
			52	52		
5	C	20	Total	O	0	0
			20	20		

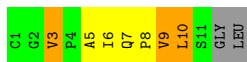
### 3 Residue-property plots [i](#)

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.

Note EDS was not executed.

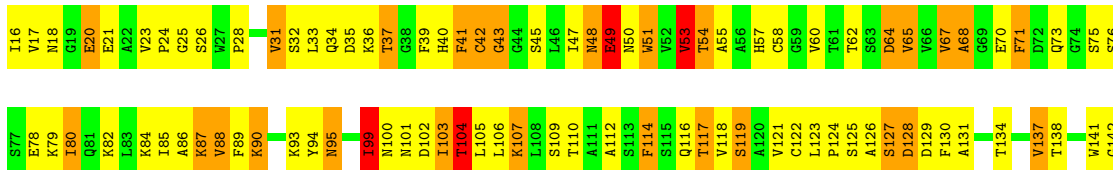
#### • Molecule 1: GAMMA-CHYMOTRYPSIN

Chain A: 



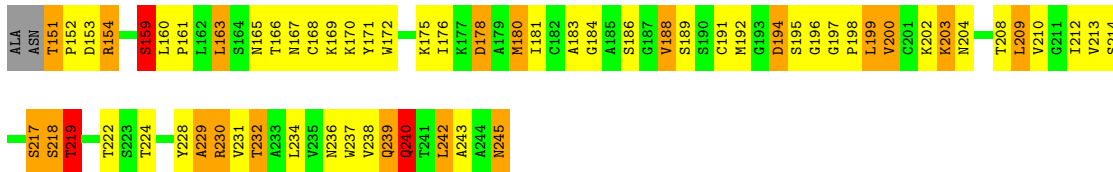
#### • Molecule 2: GAMMA-CHYMOTRYPSIN

Chain B: 



#### • Molecule 3: GAMMA-CHYMOTRYPSIN

Chain C: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.70 Å 69.70 Å 97.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.06	0/70	2.23	4/97 (4.1%)
2	B	1.19	4/999 (0.4%)	2.38	59/1361 (4.3%)
3	C	1.15	2/701 (0.3%)	2.12	28/955 (2.9%)
All	All	1.17	6/1770 (0.3%)	2.27	91/2413 (3.8%)

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	0	1
2	B	0	1
3	C	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	49	GLU	CD-OE2	6.64	1.32	1.25
2	B	78	GLU	CD-OE2	5.98	1.32	1.25
3	C	184	GLY	N-CA	-5.88	1.37	1.46
2	B	70	GLU	CD-OE2	5.73	1.31	1.25
3	C	198	PRO	N-CD	5.63	1.55	1.47
2	B	20	GLU	CD-OE2	5.03	1.31	1.25

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	154	ARG	NE-CZ-NH1	12.43	126.52	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	146	TYR	CB-CG-CD1	-12.34	113.60	121.00
2	B	128	ASP	CB-CG-OD2	-10.50	108.85	118.30
3	C	154	ARG	NE-CZ-NH2	-10.48	115.06	120.30
2	B	94	TYR	CB-CG-CD2	10.38	127.23	121.00
2	B	94	TYR	CB-CG-CD1	-10.28	114.83	121.00
2	B	36	LYS	CA-CB-CG	9.88	135.15	113.40
2	B	146	TYR	CA-C-O	9.88	140.84	120.10
2	B	60	VAL	CA-CB-CG2	9.19	124.68	110.90
2	B	101	ASN	C-N-CA	8.89	143.92	121.70
3	C	204	ASN	CA-CB-CG	8.86	132.88	113.40
3	C	183	ALA	C-N-CA	8.85	140.89	122.30
2	B	146	TYR	CA-CB-CG	-8.48	97.28	113.40
2	B	68	ALA	CB-CA-C	8.21	122.42	110.10
3	C	163	LEU	CA-CB-CG	7.82	133.28	115.30
2	B	102	ASP	CB-CG-OD1	-7.64	111.42	118.30
2	B	53	VAL	CB-CA-C	-7.32	97.49	111.40
2	B	70	GLU	OE1-CD-OE2	7.20	131.94	123.30
2	B	21	GLU	OE1-CD-OE2	7.17	131.91	123.30
2	B	43	GLY	CA-C-O	-7.16	107.72	120.60
2	B	104	THR	N-CA-CB	7.08	123.76	110.30
2	B	129	ASP	CB-CG-OD2	-7.05	111.95	118.30
2	B	128	ASP	CB-CG-OD1	7.00	124.61	118.30
2	B	102	ASP	CB-CG-OD2	6.88	124.49	118.30
2	B	107	LYS	CB-CA-C	6.87	124.14	110.40
2	B	60	VAL	CG1-CB-CG2	-6.72	100.14	110.90
2	B	88	VAL	CA-CB-CG2	-6.64	100.94	110.90
2	B	129	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	7	GLN	CB-CA-C	6.56	123.52	110.40
2	B	64	ASP	CB-CG-OD1	6.49	124.14	118.30
3	C	245	ASN	CA-C-O	-6.22	107.04	120.10
2	B	45	SER	N-CA-CB	6.21	119.81	110.50
2	B	121	VAL	CA-CB-CG1	6.20	120.19	110.90
3	C	151	THR	CA-CB-OG1	-6.17	96.03	109.00
2	B	71	PHE	N-CA-CB	6.11	121.61	110.60
3	C	232	THR	N-CA-CB	-6.11	98.69	110.30
2	B	65	VAL	CB-CA-C	6.11	123.00	111.40
2	B	114	PHE	N-CA-CB	6.01	121.42	110.60
2	B	18	ASN	C-N-CA	5.95	134.79	122.30
3	C	218	SER	O-C-N	-5.94	113.19	122.70
2	B	126	ALA	O-C-N	5.93	132.19	122.70
3	C	180	MET	CG-SD-CE	5.92	109.67	100.20
2	B	101	ASN	O-C-N	-5.85	113.33	122.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	GLU	CB-CA-C	-5.79	98.81	110.40
2	B	21	GLU	CG-CD-OE2	-5.79	106.72	118.30
3	C	218	SER	CA-CB-OG	5.79	126.82	111.20
3	C	229	ALA	CB-CA-C	5.77	118.76	110.10
2	B	80	ILE	CB-CA-C	-5.77	100.07	111.60
3	C	199	LEU	N-CA-CB	5.75	121.90	110.40
2	B	95	ASN	CA-C-N	-5.68	104.70	117.20
3	C	178	ASP	CB-CG-OD2	-5.66	113.21	118.30
2	B	146	TYR	CB-CG-CD2	5.66	124.39	121.00
2	B	138	THR	CA-CB-OG1	-5.64	97.14	109.00
3	C	151	THR	N-CA-CB	-5.64	99.59	110.30
3	C	230	ARG	NE-CZ-NH2	-5.63	117.48	120.30
3	C	236	ASN	CB-CA-C	5.63	121.67	110.40
1	A	7	GLN	CG-CD-OE1	5.62	132.83	121.60
1	A	3	VAL	CA-CB-CG1	5.58	119.27	110.90
3	C	194	ASP	CB-CG-OD1	5.55	123.29	118.30
2	B	49	GLU	CB-CG-CD	5.52	129.11	114.20
2	B	95	ASN	CA-C-O	5.52	131.69	120.10
2	B	119	SER	CB-CA-C	5.47	120.49	110.10
2	B	102	ASP	CA-C-N	-5.45	105.21	117.20
2	B	104	THR	O-C-N	5.42	131.38	122.70
2	B	144	THR	N-CA-CB	5.42	120.59	110.30
2	B	117	THR	CA-C-O	-5.41	108.73	120.10
3	C	218	SER	C-N-CA	5.37	135.12	121.70
3	C	188	VAL	CA-CB-CG2	5.36	118.94	110.90
3	C	159	SER	N-CA-CB	5.35	118.53	110.50
2	B	145	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	B	93	LYS	CA-CB-CG	5.29	125.05	113.40
3	C	219	THR	N-CA-CB	-5.29	100.25	110.30
2	B	87	LYS	O-C-N	-5.29	114.24	122.70
2	B	41	PHE	CB-CG-CD1	-5.28	117.10	120.80
1	A	9	VAL	CB-CA-C	-5.25	101.42	111.40
3	C	240	GLN	CA-C-O	-5.19	109.19	120.10
3	C	219	THR	O-C-N	5.18	131.00	122.70
2	B	49	GLU	CA-CB-CG	5.17	124.78	113.40
3	C	180	MET	CB-CG-SD	-5.15	96.95	112.40
2	B	31	VAL	N-CA-CB	5.15	122.83	111.50
2	B	70	GLU	CG-CD-OE2	-5.14	108.01	118.30
3	C	198	PRO	N-CA-C	5.14	125.47	112.10
2	B	78	GLU	CB-CG-CD	5.13	128.06	114.20
3	C	183	ALA	N-CA-CB	5.09	117.23	110.10
2	B	51	TRP	N-CA-CB	-5.09	101.44	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	VAL	O-C-N	5.04	130.77	122.70
2	B	138	THR	C-N-CA	5.04	134.30	121.70
2	B	67	VAL	CB-CA-C	5.03	120.95	111.40
2	B	137	VAL	CG1-CB-CG2	-5.03	102.86	110.90
2	B	112	ALA	CB-CA-C	5.02	117.64	110.10
3	C	242	LEU	O-C-N	5.02	130.73	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LEU	Mainchain
2	B	145	ARG	Sidechain
3	C	200	VAL	Mainchain

## 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	69	0	76	9	0
2	B	979	0	950	112	1
3	C	688	0	685	79	3
4	C	12	0	10	3	0
5	A	4	0	0	1	3
5	B	52	0	0	12	4
5	C	20	0	0	7	1
All	All	1824	0	1721	163	7

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 47.

All (163) 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)
2:B:31:VAL:HG12	2:B:68:ALA:HB2	1.30	1.07

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:TRP:HB2	3:C:176:ILE:HD11	1.36	1.02
2:B:90:LYS:HA	2:B:104:THR:HG22	1.38	1.01
2:B:58:CYS:HB2	5:B:271:HOH:O	1.61	1.01
3:C:230:ARG:NE	5:C:316:HOH:O	1.93	1.00
1:A:5:ALA:CB	2:B:116:GLN:HG3	1.93	0.98
3:C:239:GLN:HA	3:C:239:GLN:HE21	1.25	0.97
4:C:246:OAC:HB23	5:C:247:HOH:O	1.64	0.96
2:B:55:ALA:O	5:B:271:HOH:O	1.87	0.93
2:B:48:ASN:C	2:B:48:ASN:HD22	1.72	0.90
1:A:5:ALA:HB3	2:B:116:GLN:HG3	1.52	0.90
2:B:48:ASN:O	5:B:272:HOH:O	1.92	0.88
3:C:239:GLN:NE2	3:C:239:GLN:HA	1.91	0.83
2:B:143:LEU:HD12	3:C:192:MET:HB2	1.62	0.82
2:B:131:ALA:O	2:B:134:THR:OG1	1.99	0.81
3:C:172:TRP:HB2	3:C:176:ILE:CD1	2.12	0.80
3:C:172:TRP:CB	3:C:176:ILE:HD11	2.11	0.80
2:B:35:ASP:OD2	2:B:37:THR:HB	1.82	0.80
2:B:143:LEU:CD1	3:C:192:MET:HB2	2.13	0.79
3:C:217:SER:OG	3:C:219:THR:HG23	1.84	0.78
2:B:25:GLY:HA3	2:B:117:THR:HG22	1.66	0.76
3:C:165:ASN:N	5:C:311:HOH:O	2.08	0.76
1:A:5:ALA:N	5:A:296:HOH:O	2.17	0.76
2:B:28:PRO:HG2	2:B:119:SER:OG	1.87	0.75
2:B:31:VAL:CG1	2:B:68:ALA:HB2	2.14	0.74
2:B:90:LYS:CA	2:B:104:THR:HG22	2.17	0.74
2:B:90:LYS:HA	2:B:104:THR:CG2	2.14	0.73
2:B:34:GLN:HA	2:B:39:PHE:O	1.89	0.73
2:B:47:ILE:O	2:B:48:ASN:HB3	1.91	0.70
2:B:125:SER:HB2	2:B:128:ASP:H	1.56	0.70
2:B:80:ILE:O	2:B:80:ILE:HG13	1.89	0.70
3:C:217:SER:O	4:C:246:OAC:HZ	1.91	0.70
2:B:143:LEU:CD1	3:C:192:MET:HE2	2.22	0.69
2:B:71:PHE:O	3:C:154:ARG:HA	1.92	0.69
2:B:143:LEU:CD1	3:C:192:MET:CE	2.70	0.69
2:B:122:CYS:O	3:C:209:LEU:N	2.24	0.69
2:B:54:THR:OG1	2:B:55:ALA:N	2.24	0.68
3:C:212:ILE:HB	3:C:229:ALA:HB3	1.77	0.67
2:B:104:THR:HG21	5:B:287:HOH:O	1.96	0.66
3:C:209:LEU:HD13	3:C:231:VAL:HG21	1.76	0.66
2:B:95:ASN:O	2:B:99:ILE:N	2.27	0.66
2:B:73:GLN:HG3	3:C:153:ASP:O	1.96	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:HIS:O	2:B:58:CYS:C	2.34	0.64
2:B:144:THR:CG2	3:C:152:PRO:HG3	2.28	0.63
2:B:23:VAL:O	2:B:26:SER:OG	2.10	0.63
3:C:230:ARG:CZ	5:C:316:HOH:O	2.38	0.63
2:B:80:ILE:HD11	2:B:82:LYS:HE2	1.81	0.62
2:B:50:ASN:N	5:B:272:HOH:O	2.33	0.61
2:B:16:ILE:HA	3:C:189:SER:O	2.01	0.61
2:B:48:ASN:ND2	2:B:48:ASN:C	2.51	0.61
2:B:49:GLU:C	5:B:272:HOH:O	2.39	0.61
2:B:62:THR:HG22	2:B:88:VAL:CG2	2.31	0.60
2:B:47:ILE:CG2	2:B:123:LEU:HD21	2.31	0.60
3:C:167:ASN:O	3:C:170:LYS:HB2	2.02	0.60
2:B:68:ALA:HB1	5:B:263:HOH:O	2.01	0.59
3:C:230:ARG:NH1	5:C:316:HOH:O	2.36	0.58
1:A:5:ALA:HB1	2:B:116:GLN:HG3	1.83	0.57
2:B:49:GLU:N	2:B:49:GLU:OE2	2.27	0.56
2:B:103:ILE:HG21	3:C:234:LEU:HD13	1.86	0.56
2:B:53:VAL:HG13	2:B:105:LEU:CD2	2.36	0.55
4:C:246:OAC:CB2	5:C:247:HOH:O	2.39	0.55
3:C:191:CYS:O	3:C:194:ASP:HB2	2.05	0.55
2:B:117:THR:O	5:B:278:HOH:O	2.18	0.55
2:B:47:ILE:HG21	2:B:123:LEU:HD21	1.89	0.55
2:B:103:ILE:CG2	3:C:234:LEU:HD13	2.37	0.54
3:C:172:TRP:O	3:C:175:LYS:HG3	2.06	0.54
2:B:80:ILE:CD1	2:B:82:LYS:HE2	2.37	0.54
3:C:167:ASN:HA	3:C:170:LYS:HD2	1.89	0.54
2:B:130:PHE:CE2	3:C:203:LYS:HD3	2.43	0.53
2:B:55:ALA:H	3:C:196:GLY:HA2	1.74	0.53
2:B:146:TYR:CE1	3:C:192:MET:HE3	2.43	0.53
3:C:217:SER:OG	3:C:219:THR:CG2	2.56	0.52
2:B:33:LEU:HD12	2:B:42:CYS:HB3	1.91	0.52
2:B:48:ASN:ND2	2:B:50:ASN:H	2.08	0.52
2:B:143:LEU:HD11	3:C:192:MET:HE2	1.91	0.52
2:B:62:THR:CG2	2:B:88:VAL:CG2	2.88	0.51
2:B:114:PHE:CD1	2:B:118:VAL:HG12	2.45	0.51
2:B:103:ILE:HG13	3:C:212:ILE:HD13	1.91	0.51
2:B:143:LEU:HD12	3:C:192:MET:CE	2.39	0.51
2:B:90:LYS:HG3	2:B:104:THR:CG2	2.41	0.50
3:C:175:LYS:O	3:C:180:MET:HE1	2.12	0.50
3:C:181:ILE:HG23	3:C:181:ILE:O	2.11	0.50
2:B:144:THR:HG23	3:C:152:PRO:HG3	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:ASN:O	3:C:168:CYS:HB3	2.12	0.49
2:B:39:PHE:CE2	2:B:41:PHE:HB3	2.47	0.49
2:B:125:SER:CB	2:B:128:ASP:H	2.24	0.49
3:C:197:GLY:C	5:C:267:HOH:O	2.50	0.49
2:B:143:LEU:CD1	3:C:192:MET:HE1	2.43	0.48
2:B:40:HIS:C	2:B:40:HIS:CD2	2.86	0.48
2:B:146:TYR:HE1	3:C:192:MET:HE3	1.77	0.48
2:B:130:PHE:CD2	3:C:210:VAL:HG21	2.48	0.48
2:B:84:LYS:HG2	5:B:277:HOH:O	2.14	0.48
2:B:125:SER:HB2	2:B:128:ASP:N	2.26	0.47
3:C:238:VAL:O	3:C:242:LEU:HD12	2.14	0.47
2:B:128:ASP:HB3	2:B:130:PHE:CE1	2.49	0.47
2:B:142:GLY:O	2:B:143:LEU:C	2.52	0.47
2:B:55:ALA:N	3:C:196:GLY:HA2	2.29	0.47
3:C:172:TRP:CB	3:C:176:ILE:CD1	2.82	0.47
2:B:17:VAL:N	3:C:189:SER:O	2.46	0.47
2:B:51:TRP:HH2	2:B:89:PHE:CD1	2.33	0.47
2:B:62:THR:CG2	2:B:88:VAL:HG23	2.46	0.46
2:B:137:VAL:O	3:C:200:VAL:HG22	2.16	0.46
3:C:219:THR:OG1	3:C:219:THR:O	2.30	0.46
3:C:197:GLY:O	3:C:213:VAL:HG23	2.16	0.46
2:B:47:ILE:HG22	2:B:123:LEU:HD21	1.98	0.46
3:C:172:TRP:CZ2	3:C:224:THR:HG22	2.51	0.46
2:B:32:SER:HB2	2:B:141:TRP:CZ3	2.50	0.45
3:C:186:SER:OG	3:C:188:VAL:HG22	2.16	0.45
2:B:34:GLN:HG2	2:B:40:HIS:HA	1.98	0.45
1:A:8:PRO:HA	2:B:26:SER:HB2	1.99	0.45
3:C:161:PRO:CD	3:C:186:SER:HB3	2.47	0.45
1:A:9:VAL:HG12	1:A:10:LEU:N	2.28	0.44
2:B:23:VAL:HA	2:B:24:PRO:HD3	1.80	0.44
2:B:125:SER:C	2:B:127:SER:N	2.63	0.44
2:B:100:ASN:HD22	2:B:100:ASN:HA	1.43	0.44
3:C:242:LEU:O	3:C:243:ALA:C	2.56	0.44
3:C:238:VAL:O	3:C:242:LEU:CD1	2.66	0.44
2:B:49:GLU:HA	5:B:272:HOH:O	2.16	0.43
2:B:51:TRP:CZ3	2:B:105:LEU:HB3	2.54	0.43
1:A:6:ILE:HG21	5:B:261:HOH:O	2.19	0.43
2:B:146:TYR:HA	2:B:146:TYR:HD1	1.66	0.43
3:C:167:ASN:OD1	3:C:170:LYS:HD3	2.19	0.43
2:B:146:TYR:CE1	3:C:192:MET:CE	3.01	0.43
2:B:51:TRP:HA	2:B:106:LEU:O	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:ASN:ND2	3:C:230:ARG:HH11	2.17	0.43
2:B:146:TYR:HE1	3:C:192:MET:CE	2.32	0.43
3:C:245:ASN:ND2	3:C:245:ASN:N	2.66	0.43
2:B:144:THR:HG23	3:C:152:PRO:CG	2.49	0.43
2:B:146:TYR:C	2:B:146:TYR:CD1	2.84	0.43
2:B:88:VAL:H	2:B:88:VAL:HG23	1.51	0.43
3:C:165:ASN:ND2	3:C:230:ARG:NH1	2.67	0.43
2:B:49:GLU:CA	5:B:272:HOH:O	2.67	0.42
1:A:3:VAL:CG2	1:A:3:VAL:O	2.67	0.42
2:B:51:TRP:CH2	2:B:89:PHE:CD1	3.07	0.42
2:B:87:LYS:HB3	2:B:87:LYS:HE2	1.75	0.42
2:B:16:ILE:N	3:C:194:ASP:OD1	2.52	0.42
3:C:165:ASN:O	3:C:169:LYS:N	2.52	0.42
3:C:228:TYR:CD1	3:C:228:TYR:N	2.88	0.42
2:B:51:TRP:CH2	2:B:107:LYS:HB2	2.55	0.42
3:C:165:ASN:HD21	3:C:230:ARG:NH1	2.17	0.42
2:B:67:VAL:HG22	2:B:82:LYS:HG2	2.01	0.42
3:C:167:ASN:HA	3:C:170:LYS:CD	2.49	0.41
2:B:35:ASP:C	2:B:37:THR:N	2.72	0.41
3:C:209:LEU:HD23	3:C:209:LEU:HA	1.83	0.41
2:B:43:GLY:N	3:C:195:SER:O	2.36	0.41
2:B:103:ILE:HD13	3:C:237:TRP:HZ3	1.85	0.41
2:B:28:PRO:HB2	2:B:119:SER:N	2.35	0.41
3:C:165:ASN:HD21	3:C:230:ARG:HH11	1.67	0.41
2:B:53:VAL:HG13	2:B:105:LEU:HD23	2.03	0.41
2:B:86:ALA:HB2	2:B:109:SER:HA	2.03	0.41
2:B:103:ILE:HG13	3:C:212:ILE:CD1	2.50	0.41
2:B:43:GLY:O	3:C:196:GLY:HA3	2.21	0.41
3:C:168:CYS:O	3:C:171:TYR:HB2	2.20	0.41
2:B:100:ASN:ND2	3:C:180:MET:HG3	2.34	0.41
2:B:54:THR:HA	3:C:196:GLY:O	2.21	0.41
3:C:172:TRP:CZ2	3:C:224:THR:CG2	3.04	0.41
3:C:159:SER:O	3:C:160:LEU:HB3	2.21	0.41
2:B:116:GLN:HE21	2:B:116:GLN:HB2	1.40	0.40
3:C:154:ARG:HG2	3:C:154:ARG:H	1.43	0.40
2:B:25:GLY:CA	2:B:117:THR:HG22	2.44	0.40
2:B:35:ASP:O	2:B:37:THR:N	2.54	0.40
2:B:64:ASP:O	2:B:85:ILE:HD12	2.20	0.40
1:A:6:ILE:HD11	2:B:116:GLN:HG2	2.03	0.40

All (7) 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)
3:C:240:GLN:NE2	5:A:251:HOH:O[5_646]	0.51	1.69
5:B:273:HOH:O	5:B:273:HOH:O[2_675]	0.78	1.42
3:C:240:GLN:CD	5:A:251:HOH:O[5_646]	1.29	0.91
5:B:274:HOH:O	5:B:286:HOH:O[2_675]	1.64	0.56
2:B:82:LYS:NZ	5:B:302:HOH:O[6_476]	1.75	0.45
5:B:276:HOH:O	5:C:322:HOH:O[6_476]	1.86	0.34
3:C:240:GLN:CG	5:A:251:HOH:O[5_646]	2.07	0.13

## 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	9/13 (69%)	7 (78%)	2 (22%)	0	100	100
2	B	129/131 (98%)	116 (90%)	11 (8%)	2 (2%)	11	3
3	C	93/97 (96%)	87 (94%)	6 (6%)	0	100	100
All	All	231/241 (96%)	210 (91%)	19 (8%)	2 (1%)	20	8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	79	LYS
2	B	99	ILE

### 5.3.2 Protein sidechains [i](#)

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	8/10 (80%)	8 (100%)	0	100	100
2	B	109/109 (100%)	91 (84%)	18 (16%)	2	1
3	C	76/77 (99%)	58 (76%)	18 (24%)	1	0
All	All	193/196 (98%)	157 (81%)	36 (19%)	2	0

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	20	GLU
2	B	37	THR
2	B	42	CYS
2	B	48	ASN
2	B	49	GLU
2	B	53	VAL
2	B	54	THR
2	B	65	VAL
2	B	75	SER
2	B	76	SER
2	B	90	LYS
2	B	99	ILE
2	B	103	ILE
2	B	104	THR
2	B	110	THR
2	B	124	PRO
2	B	127	SER
2	B	145	ARG
3	C	151	THR
3	C	159	SER
3	C	163	LEU
3	C	166	THR
3	C	178	ASP
3	C	199	LEU
3	C	202	LYS
3	C	203	LYS
3	C	208	THR
3	C	209	LEU
3	C	214	SER
3	C	217	SER
3	C	218	SER
3	C	219	THR
3	C	222	THR
3	C	232	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	C	239	GLN
3	C	240	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	48	ASN
2	B	100	ASN
2	B	116	GLN
3	C	165	ASN
3	C	239	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	$\# Z  > 2$
4	OAC	C	246	3	12,12,13	3.99	7 (58%)	12,15,17	3.99	7 (58%)

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
4	OAC	C	246	3	1/1/1/2	0/4/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	246	OAC	CE1-CD1	-2.01	1.35	1.38
4	C	246	OAC	CB1-CG	3.62	1.56	1.51
4	C	246	OAC	O-C	3.70	1.35	1.19
4	C	246	OAC	OH-CD2	4.06	1.44	1.36
4	C	246	OAC	CZ-CE2	4.93	1.48	1.38
4	C	246	OAC	CA-C	7.38	1.59	1.50
4	C	246	OAC	CE2-CD2	7.64	1.53	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	246	OAC	CE2-CD2-CG	-3.35	116.07	120.40
4	C	246	OAC	CZ-CE2-CD2	-2.31	117.08	120.05
4	C	246	OAC	CB2-CA-C	-2.23	103.27	109.60
4	C	246	OAC	CD1-CG-CD2	3.38	121.93	118.18
4	C	246	OAC	O-C-CA	3.47	133.46	125.45
4	C	246	OAC	OH-CD2-CG	3.75	128.51	118.84
4	C	246	OAC	CG-CB1-CA	11.24	131.87	113.79

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	246	OAC	CA

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	246	OAC	3	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.