



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:16 PM UTC

PDB ID : 2PAD / pdb_00002pad
Title : BINDING OF CHLOROMETHYL KETONE SUBSTRATE ANALOGUES
TO CRYSTALLINE PAPAIN
Authors : Drenth, J.; Kalk, K.H.; Swen, H.M.
Deposited on : 1976-11-01
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

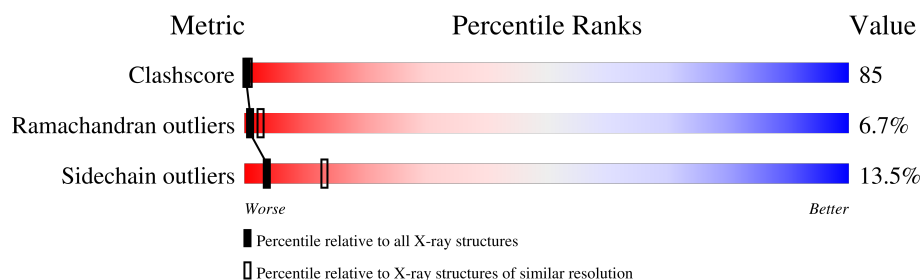
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	212	17% 54% 27% .

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	CYS	A	213	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1692 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.

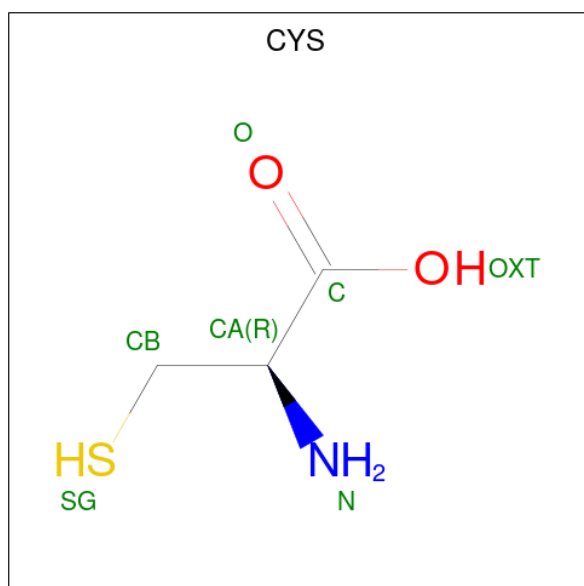
- Molecule 1 is a protein called PAPAIN.

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

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 CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	7	3	1	2	1	0	0

- Molecule 3 is water.

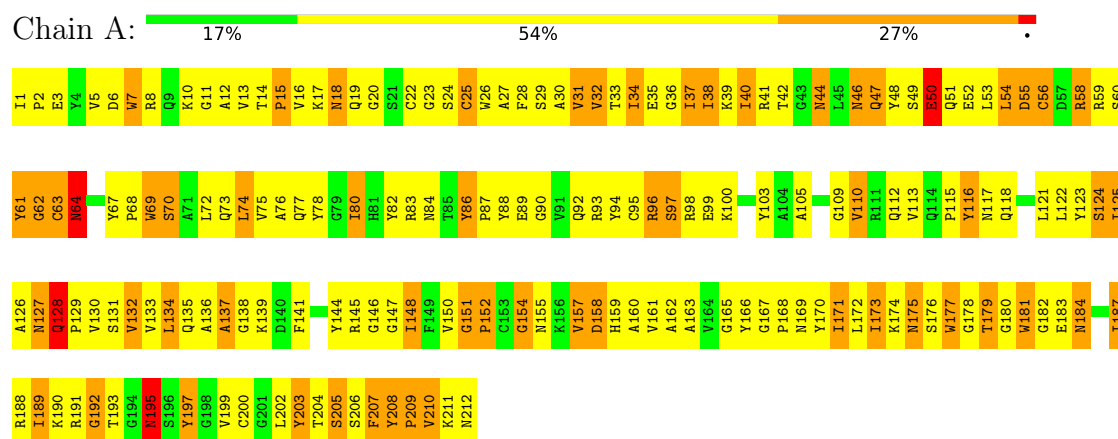
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0

3 Residue-property plots

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. 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. 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: PAPAIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.00Å 104.30Å 50.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1692	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.59	34/1699 (2.0%)	1.77	56/2306 (2.4%)

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

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	SER	N-CA	18.73	1.68	1.46
1	A	152	PRO	N-CD	-11.36	1.31	1.47
1	A	7	TRP	NE1-CE2	-8.61	1.27	1.37
1	A	69	TRP	NE1-CE2	-8.61	1.27	1.37
1	A	26	TRP	NE1-CE2	-8.59	1.28	1.37
1	A	155	ASN	CG-OD1	8.46	1.39	1.23
1	A	169	ASN	CG-OD1	8.44	1.39	1.23
1	A	175	ASN	CG-OD1	8.42	1.39	1.23
1	A	212	ASN	CG-OD1	8.42	1.39	1.23
1	A	184	ASN	CG-OD1	8.41	1.39	1.23
1	A	195	ASN	CG-OD1	8.41	1.39	1.23
1	A	84	ASN	CG-OD1	8.41	1.39	1.23
1	A	18	ASN	CG-OD1	8.38	1.39	1.23
1	A	177	TRP	NE1-CE2	-8.37	1.28	1.37
1	A	64	ASN	CG-OD1	8.37	1.39	1.23
1	A	117	ASN	CG-OD1	8.36	1.39	1.23
1	A	46	ASN	CG-OD1	8.34	1.39	1.23
1	A	44	ASN	CG-OD1	8.33	1.39	1.23
1	A	127	ASN	CG-OD1	8.33	1.39	1.23
1	A	181	TRP	NE1-CE2	-8.32	1.28	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	ASN	C-OXT	7.39	1.38	1.23
1	A	24	SER	C-N	5.74	1.41	1.33
1	A	151	GLY	C-N	-5.63	1.23	1.34
1	A	18	ASN	CG-ND2	-5.25	1.22	1.33
1	A	46	ASN	CG-ND2	-5.25	1.22	1.33
1	A	64	ASN	CG-ND2	-5.24	1.22	1.33
1	A	117	ASN	CG-ND2	-5.24	1.22	1.33
1	A	84	ASN	CG-ND2	-5.23	1.22	1.33
1	A	127	ASN	CG-ND2	-5.22	1.22	1.33
1	A	44	ASN	CG-ND2	-5.21	1.22	1.33
1	A	169	ASN	CG-ND2	-5.06	1.22	1.33
1	A	212	ASN	CG-ND2	-5.05	1.22	1.33
1	A	195	ASN	CG-ND2	-5.05	1.22	1.33
1	A	155	ASN	CG-ND2	-5.03	1.22	1.33

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	PHE	N-CA-C	16.37	133.36	108.96
1	A	169	ASN	N-CA-C	10.59	128.00	114.56
1	A	70	SER	N-CA-C	8.53	120.35	111.14
1	A	208	TYR	N-CA-C	8.36	128.29	109.81
1	A	154	GLY	N-CA-C	7.75	123.51	112.81
1	A	69	TRP	CA-C-N	-7.69	109.98	120.44
1	A	69	TRP	C-N-CA	-7.69	109.98	120.44
1	A	1	ILE	N-CA-C	-7.44	90.16	111.00
1	A	46	ASN	N-CA-C	7.31	120.56	109.23
1	A	151	GLY	O-C-N	7.20	128.97	121.77
1	A	173	ILE	N-CA-C	6.96	118.15	108.12
1	A	60	SER	N-CA-C	-6.88	100.28	110.46
1	A	116	TYR	N-CA-C	6.28	120.03	111.17
1	A	24	SER	N-CA-C	6.14	121.81	112.54
1	A	207	PHE	CB-CA-C	-5.92	97.65	111.09
1	A	179	THR	N-CA-C	-5.89	106.43	113.21
1	A	158	ASP	N-CA-C	5.82	123.20	110.80
1	A	82	TYR	N-CA-C	-5.81	103.26	110.41
1	A	210	VAL	N-CA-C	-5.75	99.54	108.44
1	A	103	TYR	N-CA-C	-5.72	103.16	110.53
1	A	84	ASN	CB-CG-ND2	5.69	124.93	116.40
1	A	64	ASN	CB-CG-ND2	5.69	124.93	116.40
1	A	18	ASN	CB-CG-ND2	5.68	124.92	116.40
1	A	169	ASN	CB-CG-ND2	5.68	124.92	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ASN	CB-CG-ND2	5.67	124.91	116.40
1	A	175	ASN	CB-CG-ND2	5.67	124.91	116.40
1	A	117	ASN	CB-CG-ND2	5.67	124.90	116.40
1	A	50	GLU	N-CA-C	-5.67	105.48	112.90
1	A	212	ASN	CB-CG-ND2	5.66	124.89	116.40
1	A	195	ASN	CB-CG-ND2	5.66	124.89	116.40
1	A	155	ASN	CB-CG-ND2	5.66	124.88	116.40
1	A	189	ILE	N-CA-C	-5.64	100.45	109.20
1	A	127	ASN	CB-CG-ND2	5.64	124.86	116.40
1	A	184	ASN	CB-CG-ND2	5.62	124.83	116.40
1	A	44	ASN	CB-CG-ND2	5.61	124.82	116.40
1	A	169	ASN	CB-CA-C	-5.60	100.40	109.13
1	A	197	TYR	N-CA-C	-5.58	104.58	111.33
1	A	177	TRP	N-CA-C	-5.56	101.95	109.95
1	A	3	GLU	N-CA-C	-5.44	106.48	113.23
1	A	84	ASN	N-CA-C	-5.39	106.76	113.55
1	A	205	SER	N-CA-C	5.33	116.88	107.61
1	A	25	CYS	CA-C-N	5.29	127.37	120.28
1	A	25	CYS	C-N-CA	5.29	127.37	120.28
1	A	80	ILE	CA-CB-CG2	-5.16	101.72	110.50
1	A	125	ILE	CA-CB-CG2	-5.16	101.73	110.50
1	A	37	ILE	CA-CB-CG2	-5.15	101.74	110.50
1	A	38	ILE	CA-CB-CG2	-5.15	101.75	110.50
1	A	40	ILE	CA-CB-CG2	-5.14	101.75	110.50
1	A	1	ILE	CA-CB-CG2	-5.14	101.77	110.50
1	A	148	ILE	CA-CB-CG2	-5.12	101.79	110.50
1	A	34	ILE	CA-CB-CG2	-5.11	101.82	110.50
1	A	189	ILE	CA-CB-CG2	-5.06	101.91	110.50
1	A	171	ILE	CA-CB-CG2	-5.05	101.91	110.50
1	A	25	CYS	O-C-N	-5.05	115.77	122.33
1	A	173	ILE	CA-CB-CG2	-5.03	101.95	110.50
1	A	187	ILE	CA-CB-CG2	-5.01	101.97	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	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	273	9
2	A	7	0	3	11	0
3	A	30	0	0	11	0
All	All	1692	0	1598	276	9

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 85.

All (276) 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:112:GLN:HB2	1:A:207:PHE:CE2	1.20	1.70
2:A:213:CYS:C	2:A:213:CYS:CA	1.75	1.57
1:A:70:SER:N	1:A:70:SER:CA	1.68	1.49
1:A:159:HIS:ND1	2:A:213:CYS:HB2	1.29	1.48
1:A:159:HIS:ND1	2:A:213:CYS:CB	1.91	1.32
1:A:112:GLN:CB	1:A:207:PHE:CE2	2.12	1.30
1:A:159:HIS:CE1	2:A:213:CYS:HB2	1.75	1.20
1:A:144:TYR:CD1	1:A:182:GLY:HA2	1.82	1.15
1:A:14:THR:HB	1:A:15:PRO:HD2	1.21	1.12
1:A:39:LYS:O	1:A:39:LYS:HD3	1.52	1.09
1:A:31:VAL:HG11	1:A:50:GLU:HG3	1.10	1.07
1:A:19:GLN:O	1:A:88:TYR:OH	1.73	1.05
1:A:135:GLN:OE1	1:A:154:GLY:N	1.88	1.03
1:A:51:GLN:OE1	1:A:89:GLU:HG2	1.58	1.03
1:A:34:ILE:O	1:A:37:ILE:HG22	1.57	1.02
1:A:132:VAL:HG11	1:A:202:LEU:CD1	1.90	1.02
1:A:112:GLN:HB2	1:A:207:PHE:CD2	2.00	0.96
1:A:144:TYR:CD1	1:A:182:GLY:CA	2.50	0.94
1:A:34:ILE:CD1	1:A:75:VAL:HG21	1.97	0.94
1:A:54:LEU:HD21	1:A:62:GLY:HA3	1.49	0.94
1:A:136:ALA:C	1:A:138:GLY:H	1.64	0.94
1:A:54:LEU:HD21	1:A:62:GLY:CA	1.97	0.93
2:A:213:CYS:C	2:A:213:CYS:CB	2.42	0.93
1:A:132:VAL:CG1	1:A:202:LEU:HD12	1.98	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:CB	1:A:15:PRO:HD2	1.96	0.92
1:A:54:LEU:HD13	1:A:92:GLN:HA	1.52	0.92
1:A:146:GLY:HA2	1:A:183:GLU:HG3	1.51	0.92
1:A:144:TYR:CE1	1:A:182:GLY:CA	2.53	0.92
1:A:69:TRP:C	1:A:70:SER:CA	2.44	0.91
1:A:136:ALA:C	1:A:138:GLY:N	2.24	0.90
1:A:31:VAL:HG11	1:A:50:GLU:CG	2.00	0.89
1:A:132:VAL:HG11	1:A:202:LEU:HD11	1.54	0.89
1:A:98:ARG:H	1:A:98:ARG:HD2	1.38	0.88
1:A:30:ALA:O	1:A:33:THR:OG1	1.90	0.88
1:A:27:ALA:O	1:A:31:VAL:CG1	2.22	0.88
1:A:112:GLN:CB	1:A:207:PHE:HE2	1.68	0.87
1:A:54:LEU:CD2	1:A:62:GLY:CA	2.51	0.86
1:A:36:GLY:O	1:A:40:ILE:HG12	1.75	0.86
1:A:63:CYS:O	1:A:64:ASN:HB3	1.76	0.85
1:A:168:PRO:HA	1:A:191:ARG:HH11	1.42	0.85
1:A:29:SER:O	1:A:33:THR:HG23	1.75	0.84
1:A:197:TYR:O	1:A:203:TYR:HB2	1.78	0.83
1:A:54:LEU:HD23	1:A:62:GLY:HA2	1.60	0.82
1:A:31:VAL:O	1:A:35:GLU:HB2	1.79	0.82
1:A:132:VAL:HG11	1:A:202:LEU:HD12	1.57	0.82
1:A:54:LEU:CD2	1:A:62:GLY:HA3	2.10	0.82
1:A:14:THR:HB	1:A:15:PRO:CD	2.08	0.81
1:A:144:TYR:CE1	1:A:182:GLY:HA2	2.14	0.81
1:A:51:GLN:OE1	1:A:89:GLU:CG	2.28	0.80
1:A:136:ALA:O	1:A:138:GLY:N	2.13	0.80
1:A:37:ILE:HG23	1:A:38:ILE:N	1.94	0.80
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.43	0.80
1:A:11:GLY:O	3:A:219:HOH:O	1.99	0.80
1:A:27:ALA:O	1:A:31:VAL:HG13	1.81	0.80
1:A:159:HIS:ND1	2:A:213:CYS:HB3	1.94	0.80
1:A:109:GLY:O	1:A:209:PRO:HA	1.82	0.79
1:A:37:ILE:CG2	1:A:38:ILE:N	2.46	0.78
1:A:148:ILE:HD13	1:A:188:ARG:HB2	1.63	0.77
1:A:202:LEU:HD23	1:A:203:TYR:HE2	1.47	0.77
1:A:98:ARG:HD2	1:A:98:ARG:N	2.00	0.77
1:A:28:PHE:O	1:A:32:VAL:HG12	1.85	0.77
1:A:29:SER:O	1:A:32:VAL:HG13	1.85	0.76
1:A:40:ILE:HG22	1:A:40:ILE:O	1.83	0.76
1:A:202:LEU:C	1:A:203:TYR:HD2	1.93	0.76
1:A:144:TYR:CE1	1:A:182:GLY:HA3	2.20	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:HB3	3:A:226:HOH:O	1.85	0.75
1:A:34:ILE:HD11	1:A:75:VAL:HG21	1.68	0.75
1:A:54:LEU:CD2	1:A:62:GLY:HA2	2.14	0.75
1:A:34:ILE:HD13	1:A:75:VAL:HG11	1.68	0.75
1:A:5:VAL:O	1:A:165:GLY:HA2	1.86	0.74
1:A:54:LEU:HD13	1:A:92:GLN:CA	2.17	0.74
1:A:5:VAL:O	1:A:165:GLY:CA	2.36	0.74
1:A:28:PHE:O	1:A:32:VAL:CG1	2.36	0.74
1:A:112:GLN:CG	1:A:207:PHE:CE2	2.71	0.74
1:A:205:SER:HA	3:A:228:HOH:O	1.89	0.72
1:A:49:SER:CB	1:A:86:TYR:HB3	2.20	0.72
1:A:41:ARG:HG3	1:A:41:ARG:HH11	1.55	0.71
1:A:51:GLN:CD	1:A:89:GLU:HG2	2.13	0.71
1:A:48:TYR:CE2	1:A:105:ALA:HB2	2.25	0.71
1:A:177:TRP:CE3	1:A:181:TRP:CD1	2.79	0.71
2:A:213:CYS:C	2:A:213:CYS:N	2.47	0.71
1:A:132:VAL:HG13	1:A:202:LEU:HD12	1.73	0.70
1:A:51:GLN:HB2	1:A:88:TYR:HA	1.72	0.70
1:A:35:GLU:CG	1:A:46:ASN:O	2.40	0.68
1:A:63:CYS:SG	1:A:90:GLY:O	2.50	0.68
1:A:35:GLU:OE2	1:A:47:GLN:HA	1.93	0.68
1:A:35:GLU:HG2	1:A:46:ASN:O	1.94	0.68
1:A:168:PRO:CA	1:A:191:ARG:HH11	2.07	0.67
1:A:27:ALA:O	1:A:31:VAL:HG12	1.94	0.67
1:A:159:HIS:CG	2:A:213:CYS:HB2	2.23	0.67
1:A:115:PRO:HB3	1:A:204:THR:O	1.95	0.67
1:A:113:VAL:CG2	1:A:208:TYR:HE1	2.07	0.67
1:A:17:LYS:HD3	1:A:83:ARG:CZ	2.25	0.67
1:A:208:TYR:O	1:A:209:PRO:O	2.13	0.66
1:A:132:VAL:CG1	1:A:202:LEU:CD1	2.61	0.66
1:A:39:LYS:HD3	1:A:39:LYS:C	2.21	0.66
1:A:125:ILE:O	1:A:125:ILE:HG22	1.94	0.66
1:A:70:SER:N	1:A:70:SER:CB	2.55	0.65
1:A:203:TYR:HD2	1:A:203:TYR:N	1.93	0.65
1:A:203:TYR:N	1:A:203:TYR:CD2	2.63	0.65
1:A:134:LEU:C	1:A:134:LEU:HD12	2.22	0.64
1:A:159:HIS:CG	2:A:213:CYS:CB	2.81	0.64
1:A:63:CYS:O	1:A:64:ASN:CB	2.45	0.64
1:A:121:LEU:O	1:A:125:ILE:HG13	1.98	0.64
1:A:177:TRP:HE3	1:A:181:TRP:CD1	2.14	0.63
1:A:202:LEU:HG	1:A:202:LEU:O	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLY:O	1:A:209:PRO:CA	2.45	0.63
1:A:96:ARG:HH11	1:A:96:ARG:CG	2.11	0.63
1:A:132:VAL:HG23	1:A:206:SER:OG	1.99	0.63
1:A:69:TRP:O	1:A:70:SER:CA	2.47	0.62
1:A:73:GLN:HA	1:A:110:VAL:HG11	1.82	0.62
1:A:113:VAL:HG22	1:A:208:TYR:HE1	1.63	0.62
1:A:39:LYS:HE2	3:A:219:HOH:O	1.99	0.61
1:A:167:GLY:O	1:A:191:ARG:NE	2.31	0.61
1:A:6:ASP:O	1:A:10:LYS:HG2	2.00	0.61
1:A:177:TRP:CZ3	1:A:181:TRP:NE1	2.68	0.61
1:A:132:VAL:CG2	1:A:206:SER:OG	2.48	0.61
1:A:18:ASN:OD1	1:A:19:GLN:N	2.34	0.61
1:A:33:THR:HG21	1:A:131:SER:HB2	1.82	0.61
1:A:7:TRP:HA	1:A:10:LYS:HB2	1.84	0.60
1:A:94:TYR:CZ	1:A:95:CYS:O	2.55	0.60
1:A:123:TYR:O	1:A:126:ALA:HB3	2.02	0.60
1:A:112:GLN:CB	1:A:207:PHE:CD2	2.74	0.60
1:A:54:LEU:CD2	1:A:92:GLN:HB2	2.32	0.60
1:A:141:PHE:CE2	1:A:181:TRP:CZ2	2.89	0.60
1:A:49:SER:HB2	1:A:86:TYR:HB3	1.84	0.60
1:A:112:GLN:CD	1:A:207:PHE:CZ	2.80	0.60
1:A:74:LEU:HD22	1:A:78:TYR:HD2	1.67	0.59
1:A:37:ILE:HD13	1:A:128:GLN:NE2	2.17	0.59
1:A:29:SER:C	1:A:32:VAL:HG13	2.28	0.59
1:A:109:GLY:O	1:A:210:VAL:N	2.36	0.59
1:A:67:TYR:O	1:A:70:SER:N	2.36	0.59
1:A:124:SER:O	1:A:128:GLN:O	2.21	0.59
1:A:135:GLN:HE22	1:A:154:GLY:HA3	1.69	0.58
1:A:55:ASP:HB3	1:A:93:ARG:O	2.03	0.58
1:A:112:GLN:HB2	1:A:207:PHE:HE2	0.79	0.57
1:A:193:THR:HG23	1:A:195:ASN:H	1.68	0.57
1:A:88:TYR:CZ	1:A:90:GLY:HA2	2.38	0.57
1:A:98:ARG:H	1:A:98:ARG:CD	2.15	0.57
1:A:11:GLY:O	1:A:39:LYS:HE2	2.05	0.57
1:A:40:ILE:O	1:A:40:ILE:CG2	2.52	0.57
1:A:144:TYR:CD1	1:A:182:GLY:HA3	2.37	0.57
1:A:168:PRO:HA	1:A:191:ARG:NH1	2.15	0.57
1:A:161:VAL:HG21	1:A:173:ILE:HG21	1.86	0.57
1:A:64:ASN:CG	1:A:64:ASN:O	2.46	0.56
1:A:144:TYR:HE1	1:A:182:GLY:HA3	1.68	0.56
1:A:2:PRO:HG2	1:A:5:VAL:HG22	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD23	1:A:62:GLY:CA	2.27	0.56
1:A:22:CYS:HB2	1:A:90:GLY:O	2.06	0.56
1:A:86:TYR:CE1	1:A:96:ARG:HB2	2.41	0.55
1:A:86:TYR:OH	1:A:96:ARG:HG3	2.06	0.55
1:A:130:VAL:HG13	1:A:207:PHE:O	2.05	0.55
1:A:38:ILE:O	1:A:42:THR:OG1	2.22	0.55
1:A:141:PHE:CE1	1:A:187:ILE:HD13	2.42	0.55
1:A:144:TYR:HD1	1:A:182:GLY:CA	2.12	0.55
1:A:118:GLN:O	1:A:122:LEU:HG	2.06	0.55
1:A:47:GLN:HG2	3:A:220:HOH:O	2.05	0.54
1:A:96:ARG:HG3	1:A:96:ARG:NH1	2.19	0.54
1:A:41:ARG:HG3	1:A:41:ARG:NH1	2.22	0.54
1:A:189:ILE:HG22	1:A:190:LYS:N	2.21	0.54
1:A:109:GLY:O	1:A:209:PRO:C	2.50	0.54
1:A:96:ARG:CG	1:A:96:ARG:NH1	2.69	0.54
1:A:34:ILE:HD13	1:A:75:VAL:HG21	1.87	0.54
1:A:52:GLU:HB2	1:A:86:TYR:CD1	2.42	0.54
1:A:98:ARG:HG2	1:A:99:GLU:N	2.22	0.54
1:A:187:ILE:HG23	1:A:187:ILE:O	2.07	0.53
1:A:127:ASN:C	1:A:128:GLN:CG	2.81	0.53
1:A:178:GLY:C	1:A:180:GLY:H	2.15	0.53
1:A:5:VAL:O	1:A:165:GLY:HA3	2.07	0.53
1:A:38:ILE:O	1:A:38:ILE:HG22	2.05	0.53
1:A:112:GLN:HA	1:A:207:PHE:CD2	2.44	0.52
1:A:116:TYR:CE1	1:A:197:TYR:HD1	2.27	0.52
1:A:86:TYR:CZ	1:A:96:ARG:HB2	2.43	0.52
1:A:80:ILE:O	1:A:80:ILE:HG23	2.09	0.52
1:A:134:LEU:HA	1:A:157:VAL:HG22	1.91	0.52
1:A:112:GLN:CA	1:A:207:PHE:CD2	2.93	0.51
1:A:118:GLN:HB2	1:A:203:TYR:CE1	2.45	0.51
1:A:118:GLN:HE22	1:A:192:GLY:H	1.58	0.51
1:A:177:TRP:HZ3	1:A:181:TRP:NE1	2.08	0.51
1:A:6:ASP:OD1	1:A:8:ARG:HB2	2.10	0.51
1:A:61:TYR:O	1:A:64:ASN:ND2	2.43	0.51
1:A:86:TYR:N	1:A:87:PRO:CD	2.73	0.51
1:A:183:GLU:O	1:A:184:ASN:HB2	2.10	0.51
1:A:134:LEU:C	1:A:134:LEU:CD1	2.84	0.51
1:A:76:ALA:HB2	3:A:240:HOH:O	2.09	0.51
1:A:135:GLN:HG2	3:A:242:HOH:O	2.10	0.51
1:A:98:ARG:HG2	1:A:99:GLU:H	1.75	0.51
1:A:177:TRP:CZ3	1:A:181:TRP:CD1	2.99	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLY:C	1:A:22:CYS:H	2.18	0.50
1:A:25:CYS:HB2	1:A:160:ALA:O	2.10	0.50
1:A:16:VAL:HB	1:A:179:THR:HG22	1.93	0.50
1:A:141:PHE:CE2	1:A:181:TRP:HZ2	2.29	0.50
1:A:183:GLU:OE1	1:A:188:ARG:HD2	2.12	0.50
1:A:48:TYR:CE2	1:A:105:ALA:CB	2.95	0.50
1:A:88:TYR:CE1	1:A:90:GLY:HA2	2.47	0.49
1:A:135:GLN:N	1:A:200:CYS:O	2.42	0.49
1:A:51:GLN:CD	1:A:89:GLU:CG	2.83	0.49
1:A:23:GLY:O	1:A:64:ASN:N	2.45	0.49
1:A:67:TYR:HB3	1:A:69:TRP:CE2	2.48	0.49
1:A:125:ILE:O	1:A:125:ILE:CG2	2.59	0.49
1:A:159:HIS:CE1	2:A:213:CYS:CB	2.64	0.49
1:A:34:ILE:O	1:A:38:ILE:HG12	2.13	0.49
1:A:96:ARG:O	1:A:100:LYS:N	2.40	0.49
1:A:19:GLN:OE1	1:A:176:SER:HB2	2.13	0.49
1:A:96:ARG:O	1:A:97:SER:C	2.56	0.48
1:A:61:TYR:N	1:A:61:TYR:CD2	2.81	0.48
1:A:67:TYR:C	1:A:69:TRP:N	2.70	0.48
1:A:74:LEU:HD22	1:A:78:TYR:CD2	2.46	0.48
1:A:17:LYS:HD3	1:A:83:ARG:NH1	2.29	0.48
1:A:37:ILE:CG2	1:A:38:ILE:H	2.24	0.48
1:A:48:TYR:O	1:A:83:ARG:HG3	2.14	0.48
1:A:64:ASN:O	1:A:64:ASN:ND2	2.47	0.48
1:A:8:ARG:C	1:A:10:LYS:H	2.21	0.47
1:A:39:LYS:C	1:A:39:LYS:CD	2.87	0.47
1:A:33:THR:OG1	1:A:72:LEU:HD21	2.14	0.47
1:A:208:TYR:C	1:A:209:PRO:O	2.58	0.47
1:A:174:LYS:HE2	3:A:224:HOH:O	2.14	0.47
1:A:54:LEU:HD22	1:A:92:GLN:HB2	1.97	0.46
1:A:171:ILE:HG13	1:A:191:ARG:HB3	1.96	0.46
1:A:33:THR:OG1	1:A:34:ILE:N	2.47	0.46
1:A:37:ILE:HG22	1:A:38:ILE:H	1.80	0.46
1:A:133:VAL:O	1:A:202:LEU:HA	2.15	0.46
1:A:151:GLY:HA3	1:A:152:PRO:HA	1.53	0.46
1:A:68:PRO:HG2	3:A:227:HOH:O	2.15	0.46
1:A:48:TYR:CZ	1:A:105:ALA:HB2	2.50	0.45
1:A:52:GLU:O	1:A:56:CYS:HB2	2.15	0.45
1:A:94:TYR:CE2	1:A:95:CYS:O	2.69	0.45
1:A:148:ILE:HA	1:A:188:ARG:O	2.17	0.45
1:A:18:ASN:OD1	1:A:20:GLY:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ARG:HA	1:A:58:ARG:HD3	1.58	0.45
1:A:38:ILE:O	1:A:38:ILE:CG2	2.59	0.45
1:A:39:LYS:O	1:A:39:LYS:CD	2.43	0.45
1:A:54:LEU:HD21	1:A:62:GLY:C	2.40	0.44
1:A:135:GLN:NE2	1:A:154:GLY:HA3	2.31	0.44
1:A:112:GLN:NE2	1:A:207:PHE:CZ	2.85	0.44
1:A:51:GLN:NE2	1:A:55:ASP:OD1	2.50	0.44
1:A:141:PHE:CE1	1:A:187:ILE:CD1	3.01	0.44
1:A:166:TYR:CD1	1:A:166:TYR:C	2.96	0.44
1:A:112:GLN:CG	1:A:207:PHE:CZ	3.01	0.44
1:A:39:LYS:CE	3:A:219:HOH:O	2.63	0.44
1:A:162:ALA:O	1:A:173:ILE:HG23	2.18	0.43
1:A:118:GLN:HB2	1:A:203:TYR:HE1	1.82	0.43
1:A:34:ILE:HD11	1:A:75:VAL:CG2	2.45	0.43
1:A:173:ILE:CG2	1:A:174:LYS:N	2.79	0.43
1:A:193:THR:HG22	3:A:237:HOH:O	2.18	0.43
1:A:162:ALA:O	1:A:174:LYS:N	2.38	0.43
1:A:41:ARG:HH11	1:A:41:ARG:CG	2.29	0.43
1:A:80:ILE:HG23	1:A:105:ALA:HB3	2.00	0.43
1:A:148:ILE:CD1	1:A:188:ARG:HB2	2.42	0.43
1:A:69:TRP:O	1:A:70:SER:HA	2.16	0.43
1:A:5:VAL:HG21	1:A:166:TYR:CE2	2.54	0.43
1:A:73:GLN:O	1:A:77:GLN:HG3	2.18	0.43
1:A:73:GLN:CA	1:A:110:VAL:HG11	2.49	0.43
1:A:159:HIS:CG	2:A:213:CYS:HB3	2.50	0.43
1:A:96:ARG:O	1:A:100:LYS:HG2	2.18	0.43
1:A:7:TRP:HB3	1:A:12:ALA:HB3	2.00	0.42
1:A:97:SER:O	1:A:100:LYS:HB2	2.19	0.42
1:A:37:ILE:HD13	1:A:128:GLN:CD	2.45	0.42
1:A:136:ALA:O	1:A:137:ALA:C	2.61	0.42
1:A:151:GLY:CA	1:A:152:PRO:C	2.88	0.42
1:A:173:ILE:HG22	1:A:174:LYS:N	2.26	0.42
1:A:41:ARG:NH1	1:A:41:ARG:CG	2.82	0.42
1:A:7:TRP:O	1:A:10:LYS:HB2	2.20	0.41
1:A:33:THR:CG2	1:A:131:SER:HB2	2.50	0.41
1:A:67:TYR:C	1:A:69:TRP:H	2.27	0.41
1:A:110:VAL:HA	1:A:209:PRO:HA	2.03	0.41
1:A:146:GLY:CA	1:A:183:GLU:HG3	2.36	0.41
1:A:144:TYR:CE2	1:A:147:GLY:N	2.89	0.41
1:A:54:LEU:CD1	1:A:92:GLN:CA	2.95	0.41
1:A:163:ALA:HA	1:A:172:LEU:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:CG2	1:A:208:TYR:CE1	2.96	0.41
1:A:189:ILE:HG22	1:A:190:LYS:H	1.86	0.41
1:A:211:LYS:HD2	1:A:211:LYS:HA	1.85	0.40
1:A:127:ASN:O	1:A:128:GLN:HG2	2.22	0.40
1:A:38:ILE:HG21	1:A:48:TYR:OH	2.22	0.40
1:A:170:TYR:CD2	1:A:170:TYR:C	2.99	0.40

All (9) 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:A:139:LYS:NZ	1:A:192:GLY:O[2_665]	1.08	1.12
1:A:41:ARG:O	1:A:77:GLN:NE2[4_565]	1.24	0.96
1:A:94:TYR:CE1	1:A:145:ARG:NH2[4_466]	1.45	0.75
1:A:94:TYR:CZ	1:A:145:ARG:NH2[4_466]	1.56	0.64
1:A:139:LYS:CE	1:A:192:GLY:O[2_665]	1.70	0.50
1:A:94:TYR:CD1	1:A:145:ARG:NH2[4_466]	1.87	0.33
1:A:139:LYS:NZ	1:A:192:GLY:C[2_665]	1.98	0.22
1:A:94:TYR:CE2	1:A:145:ARG:NH2[4_466]	2.00	0.20
1:A:94:TYR:CE1	1:A:145:ARG:CZ[4_466]	2.05	0.15

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%)	164 (78%)	32 (15%)	14 (7%)	1 3

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	209	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	62	GLY
1	A	137	ALA
1	A	195	ASN
1	A	158	ASP
1	A	192	GLY
1	A	63	CYS
1	A	97	SER
1	A	86	TYR
1	A	128	GLN
1	A	134	LEU
1	A	129	PRO
1	A	15	PRO

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%)	147 (86%)	23 (14%)	4 13

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	31	VAL
1	A	32	VAL
1	A	44	ASN
1	A	47	GLN
1	A	50	GLU
1	A	53	LEU
1	A	54	LEU
1	A	55	ASP
1	A	56	CYS
1	A	58	ARG
1	A	61	TYR
1	A	64	ASN
1	A	74	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	96	ARG
1	A	110	VAL
1	A	124	SER
1	A	128	GLN
1	A	132	VAL
1	A	150	VAL
1	A	157	VAL
1	A	199	VAL
1	A	203	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	118	GLN
1	A	127	ASN
1	A	128	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 oligosaccharides 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	$\# Z > 2$
2	CYS	A	213	1	5,6,6	4.17	3 (60%)	3,7,7	8.61	2 (66%)

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	CYS	A	213	1	-	2/6/6/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	213	CYS	CB-SG	6.57	1.95	1.81
2	A	213	CYS	CB-CA	-6.26	1.46	1.53
2	A	213	CYS	OXT-C	-2.05	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	213	CYS	CB-CA-C	-12.61	97.33	109.89
2	A	213	CYS	CA-CB-SG	-7.87	97.57	114.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	213	CYS	N-CA-CB-SG
2	A	213	CYS	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	213	CYS	11	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.