Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2016 – 12:03 AM GMT

PDB ID	:	9PAP
Title	:	STRUCTURE OF PAPAIN REFINED AT 1.65 ANGSTROMS RESOLUTION
Authors	:	Kamphuis, I.G.; Drenth, J.
Deposited on	:	1986-03-31
Resolution	:	1.65 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
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:

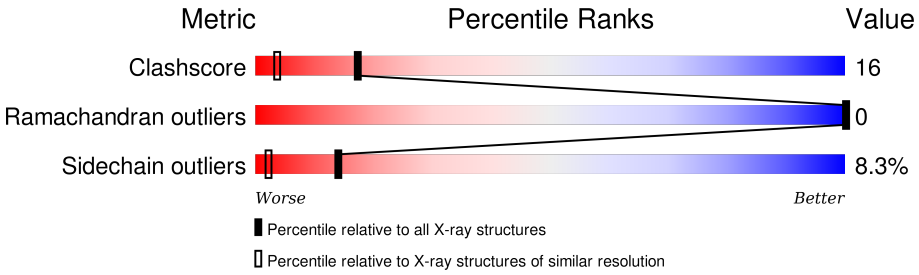
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	212	55% 33% 9% •

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	MOH	A	216	-	-	X	-
2	MOH	A	230	-	-	X	-
2	MOH	A	239	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1908 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.

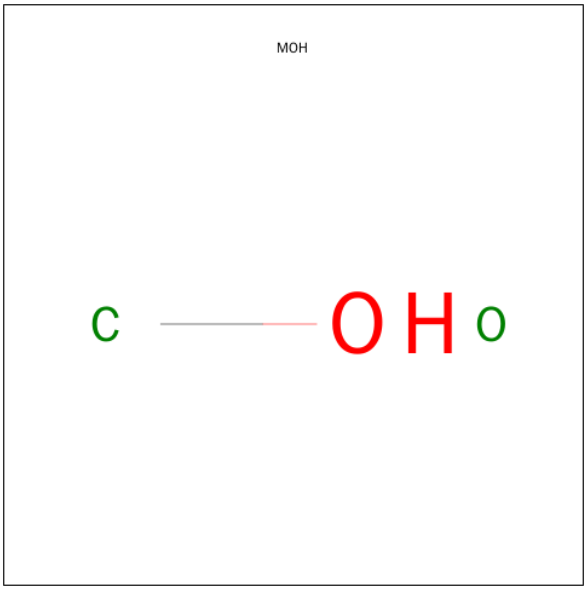
- Molecule 1 is a protein called PAPAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1655	1048	292	308	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 METHANOL (three-letter code: MOH) (formula: CH_4O).



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

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	195	Total O 195 195	0	0

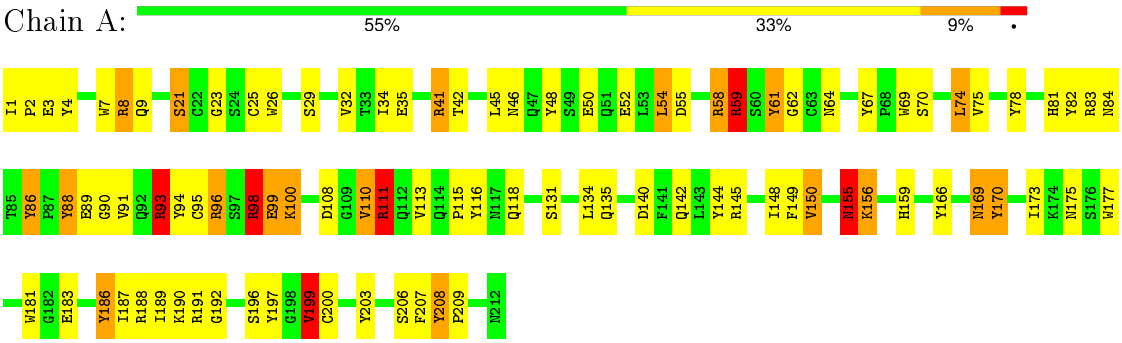
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 (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: PAPAIN

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	45.20Å 104.64Å 50.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.65	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.161 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1908	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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: OCS, 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	1.56	20/1689 (1.2%)	2.26	88/2292 (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	4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	TRP	NE1-CE2	-7.31	1.28	1.37
1	A	26	TRP	NE1-CE2	-7.14	1.28	1.37
1	A	52	GLU	CD-OE2	-6.89	1.18	1.25
1	A	99	GLU	CG-CD	6.82	1.62	1.51
1	A	86	TYR	CD1-CE1	6.42	1.49	1.39
1	A	170	TYR	CD1-CE1	6.09	1.48	1.39
1	A	183	GLU	CD-OE2	-6.04	1.19	1.25
1	A	88	TYR	CD1-CE1	6.03	1.48	1.39
1	A	166	TYR	CD1-CE1	6.01	1.48	1.39
1	A	7	TRP	CD1-NE1	5.87	1.48	1.38
1	A	177	TRP	NE1-CE2	-5.79	1.30	1.37
1	A	69	TRP	CD1-NE1	5.71	1.47	1.38
1	A	4	TYR	CD1-CE1	5.65	1.47	1.39
1	A	186	TYR	CD1-CE1	5.62	1.47	1.39
1	A	181	TRP	NE1-CE2	-5.61	1.30	1.37
1	A	3	GLU	CD-OE2	-5.35	1.19	1.25
1	A	94	TYR	CA-CB	5.28	1.65	1.53
1	A	183	GLU	CD-OE1	-5.25	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	TRP	NE1-CE2	-5.22	1.30	1.37
1	A	116	TYR	CD1-CE1	5.17	1.47	1.39

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	ARG	NE-CZ-NH1	-15.18	112.71	120.30
1	A	166	TYR	CB-CG-CD1	-14.24	112.46	121.00
1	A	108	ASP	CB-CG-OD1	13.55	130.50	118.30
1	A	67	TYR	CB-CG-CD2	-11.99	113.81	121.00
1	A	183	GLU	OE1-CD-OE2	11.92	137.60	123.30
1	A	83	ARG	NE-CZ-NH2	-11.71	114.44	120.30
1	A	8	ARG	NE-CZ-NH2	11.62	126.11	120.30
1	A	170	TYR	CB-CG-CD1	-11.32	114.20	121.00
1	A	8	ARG	NE-CZ-NH1	-10.12	115.24	120.30
1	A	145	ARG	CD-NE-CZ	9.82	137.34	123.60
1	A	48	TYR	CB-CG-CD1	-9.26	115.45	121.00
1	A	3	GLU	OE1-CD-OE2	9.17	134.31	123.30
1	A	61	TYR	CB-CG-CD1	-8.83	115.70	121.00
1	A	32	VAL	CA-CB-CG2	8.09	123.03	110.90
1	A	99	GLU	CG-CD-OE1	-8.08	102.14	118.30
1	A	145	ARG	NH1-CZ-NH2	7.91	128.10	119.40
1	A	149	PHE	CB-CG-CD1	-7.88	115.28	120.80
1	A	186	TYR	CB-CG-CD1	-7.78	116.33	121.00
1	A	82	TYR	CB-CG-CD1	-7.70	116.38	121.00
1	A	111	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	84	ASN	CA-CB-CG	-7.59	96.70	113.40
1	A	186	TYR	CG-CD1-CE1	-7.41	115.37	121.30
1	A	169	ASN	CB-CG-OD1	7.36	136.32	121.60
1	A	52	GLU	OE1-CD-OE2	7.36	132.13	123.30
1	A	88	TYR	CB-CG-CD1	-7.16	116.71	121.00
1	A	155	ASN	CA-CB-CG	7.15	129.14	113.40
1	A	108	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	35	GLU	OE1-CD-OE2	7.05	131.76	123.30
1	A	188	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	A	9	GLN	CA-CB-CG	-6.89	98.25	113.40
1	A	9	GLN	CB-CG-CD	6.83	129.37	111.60
1	A	89	GLU	OE1-CD-OE2	6.82	131.48	123.30
1	A	98	ARG	CD-NE-CZ	6.75	133.05	123.60
1	A	199	VAL	CA-CB-CG2	6.73	120.99	110.90
1	A	94	TYR	CA-CB-CG	-6.70	100.66	113.40
1	A	59	ARG	CB-CG-CD	6.69	128.99	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	GLY	O-C-N	6.61	133.28	122.70
1	A	110	VAL	CA-CB-CG1	6.54	120.70	110.90
1	A	83	ARG	NH1-CZ-NH2	6.51	126.56	119.40
1	A	45	LEU	CB-CG-CD2	-6.51	99.93	111.00
1	A	108	ASP	CA-CB-CG	-6.51	99.08	113.40
1	A	166	TYR	CB-CG-CD2	6.47	124.88	121.00
1	A	93	ARG	CA-CB-CG	6.45	127.59	113.40
1	A	41	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	59	ARG	CG-CD-NE	6.32	125.08	111.80
1	A	142	GLN	CA-CB-CG	-6.27	99.61	113.40
1	A	58	ARG	CB-CG-CD	6.04	127.32	111.60
1	A	55	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	41	ARG	CG-CD-NE	-5.97	99.26	111.80
1	A	4	TYR	CZ-CE2-CD2	-5.90	114.49	119.80
1	A	86	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	A	84	ASN	N-CA-CB	-5.89	100.00	110.60
1	A	89	GLU	CG-CD-OE1	-5.83	106.64	118.30
1	A	115	PRO	N-CA-CB	5.81	110.27	103.30
1	A	113	VAL	CG1-CB-CG2	5.76	120.12	110.90
1	A	207	PHE	CB-CG-CD1	-5.71	116.80	120.80
1	A	175	ASN	CB-CG-OD1	5.70	133.00	121.60
1	A	203	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	A	170	TYR	CG-CD1-CE1	-5.66	116.77	121.30
1	A	29	SER	N-CA-CB	-5.63	102.06	110.50
1	A	177	TRP	CD2-CE3-CZ3	-5.61	111.50	118.80
1	A	100	LYS	CD-CE-NZ	-5.59	98.84	111.70
1	A	150	VAL	CA-CB-CG1	5.58	119.27	110.90
1	A	116	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	A	32	VAL	CG1-CB-CG2	5.54	119.77	110.90
1	A	41	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	84	ASN	CB-CA-C	-5.47	99.47	110.40
1	A	208	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	A	177	TRP	NE1-CE2-CZ2	-5.44	124.42	130.40
1	A	70	SER	N-CA-CB	-5.43	102.35	110.50
1	A	197	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	A	144	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	A	50	GLU	OE1-CD-OE2	5.30	129.66	123.30
1	A	99	GLU	CG-CD-OE2	5.25	128.80	118.30
1	A	203	TYR	CG-CD1-CE1	-5.24	117.11	121.30
1	A	111	ARG	CG-CD-NE	-5.18	100.91	111.80
1	A	96	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	42	THR	CA-CB-CG2	-5.16	105.18	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48	TYR	CD1-CG-CD2	5.15	123.57	117.90
1	A	67	TYR	CG-CD1-CE1	-5.15	117.18	121.30
1	A	94	TYR	N-CA-CB	-5.14	101.35	110.60
1	A	67	TYR	CZ-CE2-CD2	-5.05	115.25	119.80
1	A	8	ARG	CB-CG-CD	-5.04	98.50	111.60
1	A	140	ASP	O-C-N	5.04	130.76	122.70
1	A	144	TYR	CG-CD1-CE1	-5.03	117.28	121.30
1	A	3	GLU	CG-CD-OE1	-5.02	108.27	118.30
1	A	41	ARG	NH1-CZ-NH2	5.01	124.91	119.40
1	A	150	VAL	N-CA-CB	-5.00	100.50	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	200	CYS	Mainchain
1	A	58	ARG	Mainchain
1	A	59	ARG	Mainchain

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	1586	50	0
2	A	58	0	0	10	0
3	A	195	0	0	8	0
All	All	1908	0	1586	53	0

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 16.

All (53) 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:98:ARG:NH1	1:A:99:GLU:HG3	1.24	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:HH12	1:A:99:GLU:CG	1.51	1.23
1:A:135:GLN:HE22	1:A:156:LYS:HE2	1.14	1.09
1:A:98:ARG:NH1	1:A:99:GLU:CG	2.10	1.08
1:A:41:ARG:HH11	2:A:216:MOH:C	1.68	1.06
1:A:135:GLN:NE2	1:A:156:LYS:HE2	1.78	0.99
1:A:98:ARG:CZ	1:A:99:GLU:HG3	1.95	0.97
1:A:46:ASN:ND2	3:A:384:HOH:O	1.97	0.90
1:A:41:ARG:NH1	2:A:216:MOH:C	2.38	0.86
1:A:98:ARG:HH12	1:A:99:GLU:CD	1.79	0.85
1:A:98:ARG:HH12	1:A:99:GLU:HG3	1.00	0.81
1:A:118:GLN:HE22	1:A:192:GLY:H	1.29	0.81
1:A:41:ARG:HH22	2:A:239:MOH:C	1.96	0.79
1:A:155:ASN:HB2	3:A:374:HOH:O	1.85	0.75
2:A:225:MOH:O	3:A:282:HOH:O	2.04	0.75
1:A:189:ILE:CG2	1:A:199:VAL:HG22	2.17	0.75
1:A:148:ILE:HD12	1:A:169:ASN:ND2	2.04	0.73
1:A:96:ARG:HA	1:A:98:ARG:HH11	1.54	0.72
1:A:155:ASN:ND2	3:A:299:HOH:O	2.27	0.67
1:A:95:CYS:O	1:A:98:ARG:HD2	1.97	0.64
1:A:8:ARG:HD3	1:A:186:TYR:CZ	2.36	0.61
1:A:41:ARG:CD	3:A:426:HOH:O	2.50	0.59
1:A:41:ARG:NH2	2:A:239:MOH:C	2.66	0.58
1:A:41:ARG:HD3	3:A:426:HOH:O	2.04	0.58
1:A:134:LEU:C	1:A:134:LEU:HD12	2.25	0.57
1:A:135:GLN:NE2	1:A:156:LYS:CE	2.63	0.56
1:A:148:ILE:CD1	1:A:169:ASN:ND2	2.68	0.56
1:A:21:SER:OG	2:A:230:MOH:C	2.55	0.55
1:A:118:GLN:NE2	1:A:192:GLY:H	2.01	0.55
1:A:189:ILE:HG23	1:A:199:VAL:HG22	1.88	0.54
1:A:148:ILE:HD12	1:A:169:ASN:HD21	1.72	0.53
1:A:190:LYS:HG3	1:A:191:ARG:N	2.24	0.51
1:A:64:ASN:HD22	2:A:234:MOH:C	2.24	0.50
1:A:131:SER:O	1:A:206:SER:HA	2.12	0.49
2:A:224:MOH:C	3:A:336:HOH:O	2.61	0.48
2:A:219:MOH:C	3:A:299:HOH:O	2.61	0.48
1:A:61:TYR:O	1:A:64:ASN:HB2	2.15	0.47
1:A:34:ILE:HD13	1:A:75:VAL:HG21	1.96	0.47
1:A:95:CYS:O	1:A:98:ARG:CD	2.64	0.45
1:A:173:ILE:HB	1:A:187:ILE:HG23	1.98	0.45
1:A:208:TYR:HB2	1:A:209:PRO:HD2	1.97	0.45
1:A:1:ILE:HA	1:A:2:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:OCS:OD3	1:A:159:HIS:HA	2.17	0.44
1:A:135:GLN:HE21	1:A:156:LYS:H	1.64	0.44
1:A:81:HIS:CE1	1:A:100:LYS:HB2	2.53	0.43
1:A:96:ARG:C	1:A:98:ARG:HD3	2.40	0.42
1:A:74:LEU:HD22	1:A:78:TYR:HD2	1.84	0.42
1:A:91:VAL:HG12	1:A:93:ARG:HD3	2.02	0.42
1:A:134:LEU:O	1:A:134:LEU:HD12	2.20	0.41
1:A:21:SER:H	2:A:230:MOH:C	2.33	0.41
1:A:170:TYR:HA	1:A:189:ILE:O	2.20	0.41
1:A:54:LEU:CD2	1:A:62:GLY:HA2	2.51	0.41
1:A:88:TYR:CZ	1:A:90:GLY:HA2	2.56	0.41

There are no symmetry-related clashes.

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	209/212 (99%)	203 (97%)	6 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	168/169 (99%)	154 (92%)	14 (8%)	14 2

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	54	LEU
1	A	59	ARG
1	A	74	LEU
1	A	86	TYR
1	A	93	ARG
1	A	98	ARG
1	A	110	VAL
1	A	111	ARG
1	A	150	VAL
1	A	155	ASN
1	A	156	LYS
1	A	196	SER
1	A	199	VAL

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

Mol	Chain	Res	Type
1	A	64	ASN
1	A	73	GLN
1	A	118	GLN
1	A	135	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)

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
1	OCS	A	25	1	7,8,9	1.35	1 (14%)	7,11,13	3.37	4 (57%)

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
1	OCS	A	25	1	-	0/4/7/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	OCS	OD1-SG	2.12	1.51	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	OCS	OD1-SG-CB	-6.95	101.08	106.94
1	A	25	OCS	O-C-CA	-3.86	115.44	125.49
1	A	25	OCS	OD2-SG-OD1	-3.06	104.48	111.61
1	A	25	OCS	OD3-SG-CB	-2.14	105.14	106.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	25	OCS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

29 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	MOH	A	214	-	1,1,1	0.57	0	0,0,0	0.00	-
2	MOH	A	215	-	1,1,1	0.45	0	0,0,0	0.00	-
2	MOH	A	216	-	1,1,1	0.59	0	0,0,0	0.00	-
2	MOH	A	217	-	1,1,1	0.39	0	0,0,0	0.00	-
2	MOH	A	218	-	1,1,1	0.46	0	0,0,0	0.00	-
2	MOH	A	219	-	1,1,1	0.34	0	0,0,0	0.00	-
2	MOH	A	220	-	1,1,1	0.46	0	0,0,0	0.00	-
2	MOH	A	221	-	1,1,1	0.22	0	0,0,0	0.00	-
2	MOH	A	222	-	1,1,1	0.34	0	0,0,0	0.00	-
2	MOH	A	223	-	1,1,1	0.55	0	0,0,0	0.00	-
2	MOH	A	224	-	1,1,1	0.35	0	0,0,0	0.00	-
2	MOH	A	225	-	1,1,1	0.40	0	0,0,0	0.00	-
2	MOH	A	226	-	1,1,1	0.56	0	0,0,0	0.00	-
2	MOH	A	227	-	1,1,1	0.58	0	0,0,0	0.00	-
2	MOH	A	228	-	1,1,1	0.60	0	0,0,0	0.00	-
2	MOH	A	229	-	1,1,1	0.40	0	0,0,0	0.00	-
2	MOH	A	230	-	1,1,1	0.59	0	0,0,0	0.00	-
2	MOH	A	231	-	1,1,1	0.51	0	0,0,0	0.00	-
2	MOH	A	232	-	1,1,1	0.55	0	0,0,0	0.00	-
2	MOH	A	233	-	1,1,1	0.49	0	0,0,0	0.00	-
2	MOH	A	234	-	1,1,1	0.63	0	0,0,0	0.00	-
2	MOH	A	235	-	1,1,1	0.63	0	0,0,0	0.00	-
2	MOH	A	236	-	1,1,1	0.45	0	0,0,0	0.00	-
2	MOH	A	237	-	1,1,1	0.50	0	0,0,0	0.00	-
2	MOH	A	238	-	1,1,1	0.56	0	0,0,0	0.00	-
2	MOH	A	239	-	1,1,1	0.48	0	0,0,0	0.00	-
2	MOH	A	240	-	1,1,1	0.62	0	0,0,0	0.00	-
2	MOH	A	241	-	1,1,1	0.47	0	0,0,0	0.00	-
2	MOH	A	242	-	1,1,1	0.50	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	MOH	A	214	-	-	0/0/0/0	0/0/0/0
2	MOH	A	215	-	-	0/0/0/0	0/0/0/0
2	MOH	A	216	-	-	0/0/0/0	0/0/0/0
2	MOH	A	217	-	-	0/0/0/0	0/0/0/0
2	MOH	A	218	-	-	0/0/0/0	0/0/0/0
2	MOH	A	219	-	-	0/0/0/0	0/0/0/0
2	MOH	A	220	-	-	0/0/0/0	0/0/0/0
2	MOH	A	221	-	-	0/0/0/0	0/0/0/0
2	MOH	A	222	-	-	0/0/0/0	0/0/0/0
2	MOH	A	223	-	-	0/0/0/0	0/0/0/0
2	MOH	A	224	-	-	0/0/0/0	0/0/0/0
2	MOH	A	225	-	-	0/0/0/0	0/0/0/0
2	MOH	A	226	-	-	0/0/0/0	0/0/0/0
2	MOH	A	227	-	-	0/0/0/0	0/0/0/0
2	MOH	A	228	-	-	0/0/0/0	0/0/0/0
2	MOH	A	229	-	-	0/0/0/0	0/0/0/0
2	MOH	A	230	-	-	0/0/0/0	0/0/0/0
2	MOH	A	231	-	-	0/0/0/0	0/0/0/0
2	MOH	A	232	-	-	0/0/0/0	0/0/0/0
2	MOH	A	233	-	-	0/0/0/0	0/0/0/0
2	MOH	A	234	-	-	0/0/0/0	0/0/0/0
2	MOH	A	235	-	-	0/0/0/0	0/0/0/0
2	MOH	A	236	-	-	0/0/0/0	0/0/0/0
2	MOH	A	237	-	-	0/0/0/0	0/0/0/0
2	MOH	A	238	-	-	0/0/0/0	0/0/0/0
2	MOH	A	239	-	-	0/0/0/0	0/0/0/0
2	MOH	A	240	-	-	0/0/0/0	0/0/0/0
2	MOH	A	241	-	-	0/0/0/0	0/0/0/0
2	MOH	A	242	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	216	MOH	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	219	MOH	1	0
2	A	224	MOH	1	0
2	A	225	MOH	1	0
2	A	230	MOH	2	0
2	A	234	MOH	1	0
2	A	239	MOH	2	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.