



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 06:20 PM EDT

PDB ID : 3H09  
Title : The structure of Haemophilus influenzae IgA1 protease  
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Deposited on : 2009-04-08  
Resolution : 1.75 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

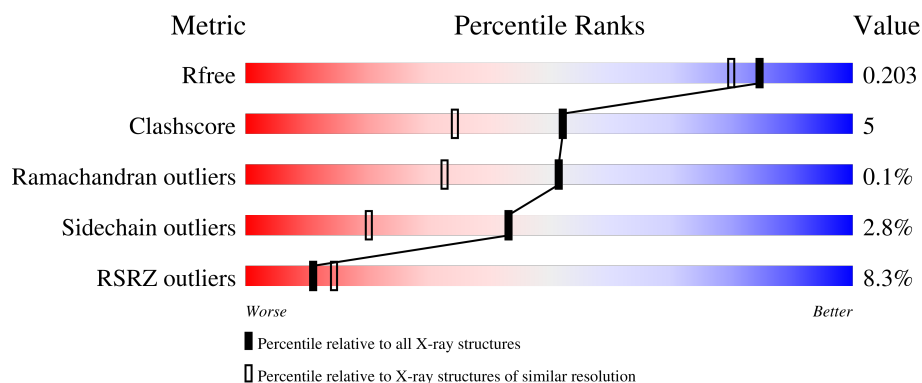
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	989	<div> <div>9%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	B	989	<div> <div>7%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17310 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 Immunoglobulin A1 protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	961	Total	C	N	O	S	0	58	0
			7718	4809	1353	1545	11			
1	B	964	Total	C	N	O	S	0	57	0
			7725	4814	1351	1549	11			

There are 12 discrepancies between the modelled and reference sequences:

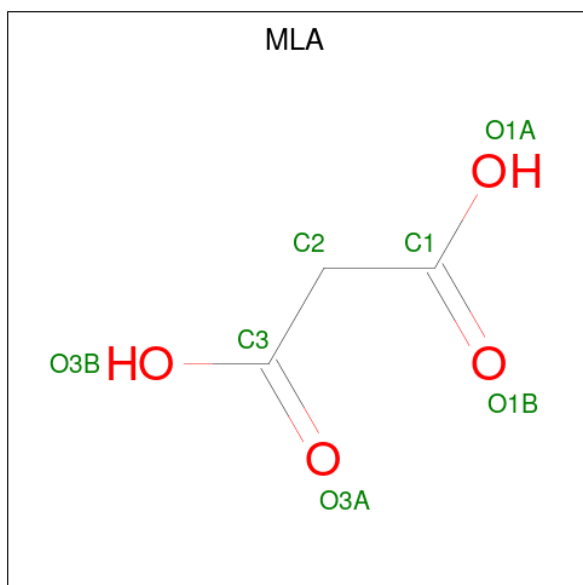
Chain	Residue	Modelled	Actual	Comment	Reference
A	1007	HIS	ASN	engineered mutation	UNP P44969
A	1008	HIS	ASN	engineered mutation	UNP P44969
A	1009	HIS	ILE	engineered mutation	UNP P44969
A	1010	HIS	GLN	engineered mutation	UNP P44969
A	1011	HIS	ALA	engineered mutation	UNP P44969
A	1012	HIS	ASP	engineered mutation	UNP P44969
B	1007	HIS	ASN	engineered mutation	UNP P44969
B	1008	HIS	ASN	engineered mutation	UNP P44969
B	1009	HIS	ILE	engineered mutation	UNP P44969
B	1010	HIS	GLN	engineered mutation	UNP P44969
B	1011	HIS	ALA	engineered mutation	UNP P44969
B	1012	HIS	ASP	engineered mutation	UNP P44969

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is MALONIC ACID (three-letter code: MLA) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 3 4	0	0
3	A	1	Total C O 7 3 4	0	0
3	A	1	Total C O 7 3 4	0	0
3	B	1	Total C O 7 3 4	0	0
3	B	1	Total C O 7 3 4	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	3	Total Na 3 3	0	0

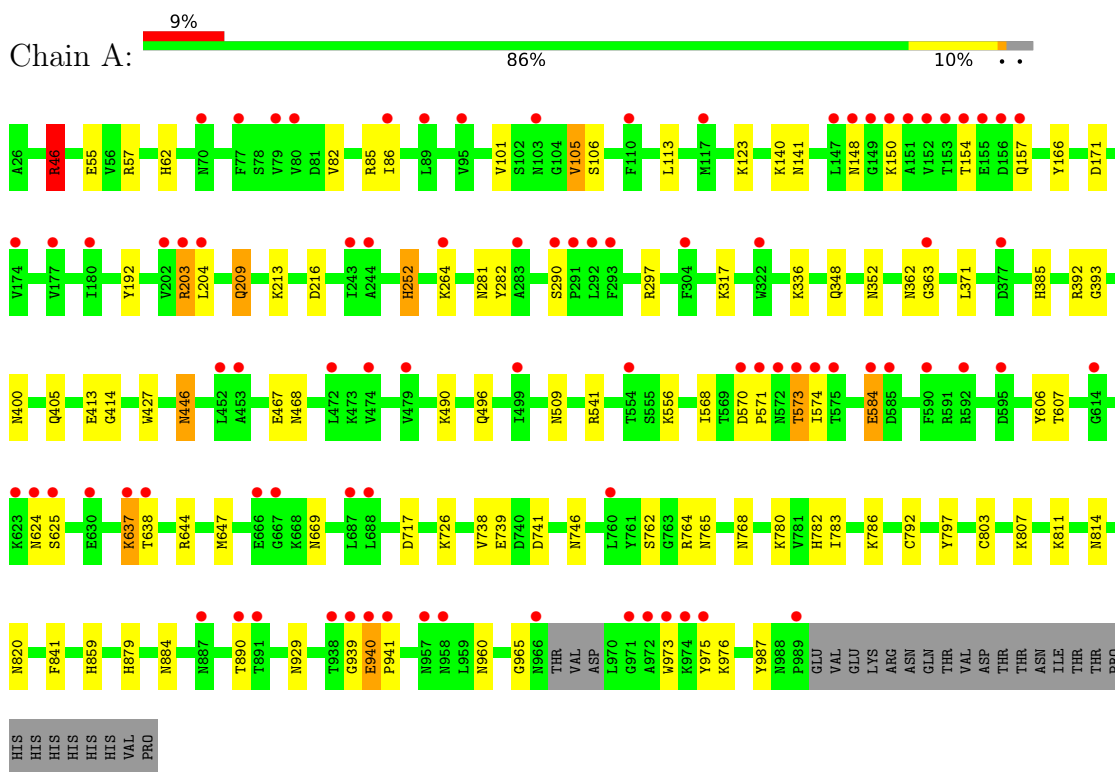
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	919	Total O 919 919	0	0
5	B	893	Total O 893 893	0	0

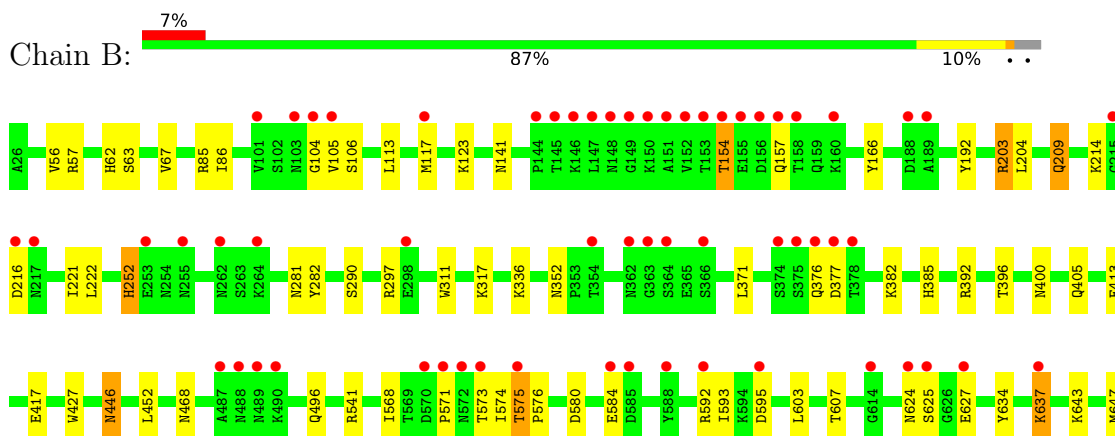
### 3 Residue-property plots [i](#)

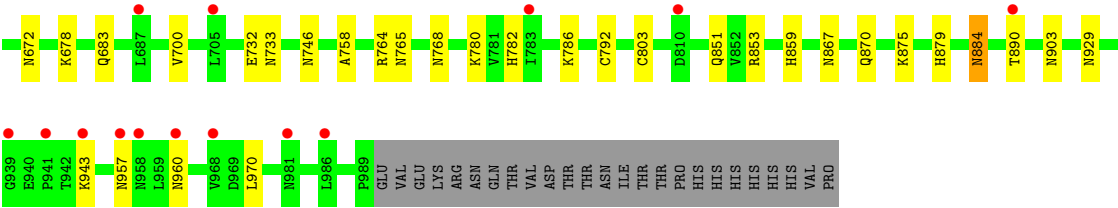
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Immunoglobulin A1 protease



- Molecule 1: Immunoglobulin A1 protease





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.39Å 131.87Å 111.81Å 90.00° 113.11° 90.00°	Depositor
Resolution (Å)	33.18 – 1.75 33.18 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.18-1.75) 99.6 (33.18-1.75)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 1.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.161 , 0.190 0.180 , 0.203	Depositor DCC
$R_{free}$ test set	12657 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17310	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, MLA, NA

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	0.67	0/8030	0.75	7/10869 (0.1%)
1	B	0.63	0/8036	0.70	0/10887
All	All	0.65	0/16066	0.72	7/21756 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	46[A]	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	46[B]	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	57	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	46[A]	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	46[B]	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	171	ASP	CB-CG-OD1	5.70	123.43	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	7718	0	7610	86	0
1	B	7725	0	7605	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	8	0	6	0	0
2	B	8	0	6	0	0
3	A	21	0	6	1	0
3	B	14	0	4	1	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
5	A	919	0	0	13	0
5	B	893	0	0	17	0
All	All	17310	0	15237	168	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 5.

All (168) 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:571:PRO:HA	1:A:647[B]:MET:SD	1.81	1.19
1:A:352[B]:ASN:ND2	5:A:1740:HOH:O	1.79	1.12
1:A:46[A]:ARG:HD3	5:A:1467:HOH:O	1.49	1.10
1:A:939:GLY:HA2	1:A:975:TYR:OH	1.58	1.03
1:B:571:PRO:HA	1:B:647[B]:MET:SD	1.99	1.03
1:A:105:VAL:HG23	1:A:140[B]:LYS:HE3	1.04	1.01
1:A:105:VAL:CG2	1:A:140[B]:LYS:HE3	1.93	0.99
1:B:672:ASN:ND2	5:B:1783:HOH:O	1.95	0.98
1:A:154:THR:HA	1:A:157:GLN:HG2	1.52	0.91
1:A:105:VAL:HG23	1:A:140[B]:LYS:CE	1.98	0.91
1:A:571:PRO:CA	1:A:647[B]:MET:SD	2.60	0.89
1:B:574:ILE:HD11	1:B:647[B]:MET:HG2	1.53	0.88
1:B:297:ARG:HH11	1:B:297:ARG:HG3	1.36	0.87
1:B:192:TYR:H	1:B:252:HIS:HD2	1.20	0.87
1:A:203:ARG:HH11	1:A:281:ASN:HD22	1.22	0.84
1:A:574:ILE:CD1	1:A:647[B]:MET:HG3	2.08	0.83
1:B:957:ASN:HB3	5:B:1603:HOH:O	1.78	0.82
1:A:574:ILE:HD11	1:A:647[B]:MET:HG3	1.63	0.81
1:B:203:ARG:HH11	1:B:281:ASN:HD22	1.27	0.80
1:A:192:TYR:H	1:A:252:HIS:HD2	1.29	0.80
1:B:571:PRO:CA	1:B:647[B]:MET:SD	2.72	0.76
1:A:574:ILE:HD11	1:A:647[B]:MET:CG	2.16	0.75
1:A:352[A]:ASN:HD21	1:A:400:ASN:HD22	1.34	0.74
1:A:644[B]:ARG:HB2	1:A:644[B]:ARG:NH1	2.01	0.74
1:A:352[B]:ASN:OD1	5:A:1813:HOH:O	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:LYS:HG2	1:B:903[B]:ASN:HD21	1.51	0.74
1:B:574:ILE:CD1	1:B:647[B]:MET:HG2	2.19	0.72
1:A:352[A]:ASN:ND2	1:A:400:ASN:HD22	1.88	0.72
3:B:2000:MLA:O1A	5:B:1061:HOH:O	2.07	0.72
1:A:392[A]:ARG:NH1	1:A:413[A]:GLU:OE1	2.23	0.71
1:A:939:GLY:CA	1:A:975:TYR:OH	2.38	0.71
1:A:413[B]:GLU:OE2	5:A:1704:HOH:O	2.07	0.71
1:B:853:ARG:NH2	5:B:1696:HOH:O	2.23	0.70
1:B:392[A]:ARG:NH1	1:B:413[A]:GLU:OE1	2.24	0.69
1:B:764:ARG:HE	1:B:765:ASN:HD22	1.37	0.69
1:B:396[A]:THR:HG22	1:B:417:GLU:HB3	1.73	0.69
3:A:2200:MLA:O3A	5:A:1825:HOH:O	2.09	0.68
1:B:929:ASN:HD21	1:B:960[A]:ASN:HD22	1.40	0.68
1:A:568:ILE:HG22	1:A:647[B]:MET:SD	2.34	0.67
1:B:625:SER:HB3	1:B:637:LYS:HE3	1.75	0.67
1:B:105:VAL:HG22	5:B:1371:HOH:O	1.93	0.67
1:B:154:THR:HA	1:B:157:GLN:HG2	1.75	0.67
1:A:940:GLU:HB2	1:A:941:PRO:HD2	1.78	0.66
1:A:405:GLN:HE21	1:A:427:TRP:HE1	1.42	0.66
1:B:607[B]:THR:HG23	1:B:634:TYR:HE1	1.60	0.65
1:B:929:ASN:ND2	1:B:960[A]:ASN:HD22	1.94	0.65
1:A:782:HIS:HD2	1:A:786:LYS:NZ	1.95	0.64
1:B:405:GLN:HE21	1:B:427:TRP:HE1	1.46	0.64
1:B:496:GLN:HE21	1:B:541:ARG:HH12	1.42	0.64
1:A:764:ARG:HE	1:A:765:ASN:HD22	1.43	0.64
1:A:879:HIS:HD2	5:A:1783:HOH:O	1.81	0.64
1:A:859:HIS:ND1	1:A:879:HIS:HE1	1.96	0.64
1:A:746:ASN:ND2	1:A:768:ASN:HD22	1.96	0.64
1:B:764:ARG:HE	1:B:765:ASN:ND2	1.96	0.63
1:A:154:THR:HA	1:A:157:GLN:CG	2.28	0.63
1:B:297:ARG:HG3	1:B:297:ARG:NH1	2.11	0.63
1:B:782:HIS:HD2	1:B:786:LYS:NZ	1.96	0.63
1:B:782:HIS:HD2	1:B:786:LYS:HZ1	1.48	0.61
1:B:764:ARG:HH21	1:B:765:ASN:HD21	1.47	0.60
1:B:56:VAL:HG23	1:B:67[B]:VAL:CG1	2.32	0.60
1:A:965:GLY:HA3	1:A:973:TRP:CD2	2.37	0.59
1:B:643:LYS:O	1:B:647[B]:MET:HG3	2.02	0.59
1:B:571:PRO:O	1:B:643:LYS:HD3	2.03	0.59
1:A:764:ARG:HE	1:A:765:ASN:ND2	2.00	0.58
1:B:405:GLN:NE2	1:B:427:TRP:HE1	2.01	0.58
1:A:929:ASN:HD22	1:A:960:ASN:HB2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLN:HE21	1:B:209:GLN:HA	1.69	0.57
1:B:746:ASN:ND2	1:B:768:ASN:HD22	2.03	0.57
1:A:371:LEU:O	1:A:385:HIS:HD2	1.87	0.56
1:A:405:GLN:NE2	1:A:427:TRP:HE1	2.02	0.56
1:B:859:HIS:ND1	1:B:879:HIS:HE1	2.02	0.56
1:A:62:HIS:HE1	5:A:1852:HOH:O	1.89	0.56
1:A:86[A]:ILE:HD12	1:A:101:VAL:HG11	1.87	0.56
1:A:570:ASP:O	1:A:573:THR:OG1	2.22	0.56
1:A:782:HIS:HD2	1:A:786:LYS:HZ1	1.52	0.56
1:A:644[B]:ARG:HB2	1:A:644[B]:ARG:HH11	1.68	0.56
1:B:123:LYS:NZ	1:B:733:ASN:HD21	2.03	0.56
1:A:584:GLU:HA	5:A:1844:HOH:O	2.05	0.56
1:B:867[A]:ASN:OD1	5:B:1871:HOH:O	2.18	0.55
1:A:385:HIS:HE1	5:A:1931:HOH:O	1.89	0.55
1:B:851[A]:GLN:NE2	1:B:870:GLN:NE2	2.55	0.55
1:A:764:ARG:HH21	1:A:765:ASN:HD21	1.54	0.55
1:A:106[A]:SER:HB2	5:A:1689:HOH:O	2.06	0.54
1:A:973:TRP:CH2	1:A:975:TYR:HB2	2.42	0.54
1:B:746:ASN:HD21	1:B:768:ASN:HD22	1.56	0.54
1:B:929:ASN:HD22	1:B:960[A]:ASN:HB2	1.71	0.54
1:B:592:ARG:HG2	1:B:593:ILE:N	2.23	0.53
1:A:746:ASN:HD21	1:A:768:ASN:HD22	1.56	0.53
1:B:192:TYR:H	1:B:252:HIS:CD2	2.12	0.53
1:B:607[B]:THR:HG23	1:B:634:TYR:CE1	2.44	0.53
1:A:568:ILE:CG2	1:A:647[B]:MET:SD	2.96	0.53
1:A:496:GLN:HE21	1:A:541:ARG:HH12	1.57	0.52
1:B:221:ILE:O	1:B:222[A]:LEU:HD23	2.09	0.52
1:A:739:GLU:OE2	1:A:811[A]:LYS:HE2	2.09	0.52
1:B:371:LEU:O	1:B:385:HIS:HD2	1.93	0.52
1:A:792:CYS:HG	1:A:803[B]:CYS:HB3	1.74	0.52
1:A:940:GLU:CB	1:A:941:PRO:HD2	2.40	0.51
1:B:929:ASN:HD22	1:B:960[B]:ASN:HB3	1.75	0.51
1:A:574:ILE:HD11	1:A:647[B]:MET:HG2	1.93	0.51
1:A:209:GLN:HA	1:A:209:GLN:HE21	1.76	0.51
1:A:574:ILE:HD12	1:A:647[B]:MET:HG3	1.92	0.51
1:B:282:TYR:CZ	1:B:317:LYS:HA	2.46	0.51
1:A:393:GLY:O	1:A:414:GLY:HA3	2.11	0.50
1:A:792:CYS:HG	1:A:803[A]:CYS:HG	0.62	0.50
1:B:376:GLN:O	1:B:382:LYS:HE3	2.12	0.50
1:A:606:TYR:O	1:A:637:LYS:HE2	2.11	0.50
1:A:571:PRO:N	1:A:647[B]:MET:SD	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLN:NE2	1:A:541:ARG:HH22	2.10	0.50
1:B:496:GLN:NE2	1:B:541:ARG:HH22	2.09	0.49
1:B:568:ILE:HG22	1:B:647[B]:MET:SD	2.52	0.49
1:B:106[B]:SER:OG	5:B:1767:HOH:O	2.19	0.49
1:B:960[A]:ASN:ND2	5:B:1269:HOH:O	2.44	0.49
1:B:56:VAL:CG2	1:B:67[B]:VAL:CG1	2.92	0.48
1:B:86[A]:ILE:HD11	1:B:104:GLY:HA3	1.96	0.48
1:B:117[B]:MET:HG3	5:B:1071:HOH:O	2.14	0.48
1:B:141:ASN:HD21	1:B:336:LYS:NZ	2.11	0.48
1:A:352[A]:ASN:HD21	1:A:400:ASN:ND2	2.09	0.47
1:B:57[A]:ARG:HG2	1:B:63:SER:HA	1.96	0.47
1:B:732[B]:GLU:HG3	5:B:1664:HOH:O	2.13	0.47
1:B:62[A]:HIS:HD2	5:B:1766:HOH:O	1.98	0.47
1:B:446:ASN:ND2	1:B:468:ASN:HD21	2.12	0.47
1:B:637:LYS:HG3	5:B:1125:HOH:O	2.15	0.47
1:B:574:ILE:CD1	1:B:647[B]:MET:CG	2.91	0.47
1:B:879:HIS:HD2	5:B:1322:HOH:O	1.96	0.47
1:A:939:GLY:HA2	1:A:975:TYR:CZ	2.47	0.47
1:A:348:GLN:O	1:A:362[A]:ASN:ND2	2.48	0.47
1:A:446:ASN:ND2	1:A:468:ASN:HD21	2.13	0.47
1:A:141:ASN:HD21	1:A:336:LYS:NZ	2.13	0.47
1:A:607:THR:HG22	1:A:637:LYS:HD2	1.97	0.47
1:A:204:LEU:O	1:A:290:SER:HB2	2.15	0.46
1:A:814:ASN:ND2	5:A:1349:HOH:O	2.43	0.45
1:A:509:ASN:ND2	5:A:1410:HOH:O	2.47	0.45
1:A:965:GLY:HA3	1:A:973:TRP:CE3	2.51	0.45
1:B:452:LEU:C	1:B:452:LEU:HD23	2.37	0.45
1:B:496:GLN:NE2	1:B:541:ARG:HH12	2.12	0.45
1:B:683[B]:GLN:NE2	5:B:1280:HOH:O	2.41	0.45
1:A:717:ASP:OD2	1:A:726:LYS:NZ	2.37	0.45
1:A:568:ILE:HG21	1:A:647[B]:MET:HG2	1.99	0.44
1:B:884:ASN:C	1:B:884:ASN:HD22	2.21	0.44
1:A:282:TYR:CZ	1:A:317:LYS:HA	2.52	0.44
1:A:82:VAL:HB	1:A:113:LEU:HD23	2.00	0.44
1:A:762[B]:SER:OG	1:A:783[B]:ILE:HA	2.18	0.44
1:B:62[A]:HIS:CD2	5:B:1843:HOH:O	2.71	0.44
1:A:297:ARG:HH11	1:A:297:ARG:HG3	1.82	0.44
1:A:46[B]:ARG:NH1	1:A:55:GLU:O	2.51	0.44
1:A:820[B]:ASN:OD1	1:A:841:PHE:CE2	2.71	0.44
1:A:738:VAL:HB	1:A:741:ASP:HB3	1.99	0.43
1:B:970:LEU:HD23	5:B:1305:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ARG:HH11	1:B:281:ASN:ND2	2.06	0.43
1:B:625:SER:CB	1:B:637:LYS:HE3	2.45	0.43
1:B:580:ASP:HA	1:B:603:LEU:HD12	2.01	0.43
1:B:113:LEU:HD21	5:B:1247:HOH:O	2.19	0.42
1:B:56:VAL:CG2	1:B:67[B]:VAL:HG12	2.49	0.42
1:B:352:ASN:ND2	1:B:400:ASN:HD22	2.17	0.42
1:A:352[B]:ASN:ND2	5:A:1444:HOH:O	2.52	0.42
1:A:976:LYS:HB2	1:A:987:TYR:CE2	2.54	0.42
1:B:624:ASN:HB2	1:B:627:GLU:HG3	2.01	0.42
1:B:792:CYS:HG	1:B:803[B]:CYS:HB3	1.85	0.41
1:A:807:LYS:HE3	1:A:807:LYS:HB2	1.88	0.41
1:B:571:PRO:N	1:B:647[B]:MET:SD	2.94	0.41
1:A:782:HIS:CD2	1:A:786:LYS:NZ	2.83	0.41
1:B:204:LEU:O	1:B:290:SER:HB2	2.20	0.41
1:B:575:THR:HA	1:B:576:PRO:HD3	1.93	0.41
1:A:467:GLU:HG3	1:A:490[A]:LYS:HB3	2.03	0.41
1:B:700:VAL:HG12	1:B:758:ALA:HB1	2.02	0.40
1:A:123:LYS:HB2	1:A:797:TYR:CZ	2.57	0.40

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	1015/989 (103%)	984 (97%)	30 (3%)	1 (0%)	51	33
1	B	1019/989 (103%)	988 (97%)	31 (3%)	0	100	100
All	All	2034/1978 (103%)	1972 (97%)	61 (3%)	1 (0%)	51	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	GLY

### 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	873/843 (104%)	846 (97%)	27 (3%)	40	17
1	B	875/843 (104%)	854 (98%)	21 (2%)	49	26
All	All	1748/1686 (104%)	1700 (97%)	48 (3%)	43	22

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46[A]	ARG
1	A	46[B]	ARG
1	A	85	ARG
1	A	105	VAL
1	A	148	ASN
1	A	150	LYS
1	A	166	TYR
1	A	203	ARG
1	A	209	GLN
1	A	213	LYS
1	A	216	ASP
1	A	252	HIS
1	A	264	LYS
1	A	446	ASN
1	A	556	LYS
1	A	573	THR
1	A	584	GLU
1	A	624	ASN
1	A	625	SER
1	A	637	LYS
1	A	638[A]	THR
1	A	638[B]	THR
1	A	669	ASN

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Mol	Chain	Res	Type
1	A	780	LYS
1	A	884	ASN
1	A	890	THR
1	A	940	GLU
1	B	85	ARG
1	B	154	THR
1	B	166	TYR
1	B	203	ARG
1	B	209	GLN
1	B	214	LYS
1	B	216	ASP
1	B	252	HIS
1	B	311	TRP
1	B	377	ASP
1	B	446	ASN
1	B	573	THR
1	B	575	THR
1	B	584	GLU
1	B	595	ASP
1	B	637	LYS
1	B	678	LYS
1	B	780	LYS
1	B	884	ASN
1	B	890	THR
1	B	943	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	103	ASN
1	A	141	ASN
1	A	209	GLN
1	A	252	HIS
1	A	281	ASN
1	A	348	GLN
1	A	350	ASN
1	A	368	ASN
1	A	385	HIS
1	A	405	GLN
1	A	446	ASN
1	A	496	GLN

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Mol	Chain	Res	Type
1	A	509	ASN
1	A	586	ASN
1	A	624	ASN
1	A	669	ASN
1	A	693	ASN
1	A	734	ASN
1	A	744	ASN
1	A	746	ASN
1	A	765	ASN
1	A	782	HIS
1	A	814	ASN
1	A	817	ASN
1	A	857	ASN
1	A	879	HIS
1	A	929	ASN
1	A	953	ASN
1	A	960	ASN
1	B	103	ASN
1	B	141	ASN
1	B	209	GLN
1	B	252	HIS
1	B	281	ASN
1	B	350	ASN
1	B	352	ASN
1	B	383	ASN
1	B	385	HIS
1	B	405	GLN
1	B	446	ASN
1	B	496	GLN
1	B	672	ASN
1	B	693	ASN
1	B	733	ASN
1	B	744	ASN
1	B	746	ASN
1	B	765	ASN
1	B	782	HIS
1	B	814	ASN
1	B	870	GLN
1	B	879	HIS
1	B	884	ASN
1	B	929	ASN
1	B	966	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	MLA	A	2200	-	0,6,6	-	-	0,7,7	-	-
2	ACT	B	1900	-	1,3,3	1.64	0	0,3,3	-	-
2	ACT	B	1700	-	1,3,3	2.27	1 (100%)	0,3,3	-	-
3	MLA	A	2100	-	0,6,6	-	-	0,7,7	-	-
3	MLA	A	2000	-	0,6,6	-	-	0,7,7	-	-
2	ACT	A	1900	-	1,3,3	2.23	1 (100%)	0,3,3	-	-
2	ACT	A	1800	-	1,3,3	2.42	1 (100%)	0,3,3	-	-
3	MLA	B	2000	-	0,6,6	-	-	0,7,7	-	-
3	MLA	B	1800	-	0,6,6	-	-	0,7,7	-	-

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
3	MLA	A	2200	-	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLA	A	2100	-	-	0/0/4/4	-
3	MLA	A	2000	-	-	0/0/4/4	-
3	MLA	B	2000	-	-	0/0/4/4	-
3	MLA	B	1800	-	-	0/0/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1800	ACT	CH3-C	2.42	1.51	1.48
2	B	1700	ACT	CH3-C	2.27	1.51	1.48
2	A	1900	ACT	CH3-C	2.23	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2200	MLA	1	0
3	B	2000	MLA	1	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

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	961/989 (97%)	0.41	85 (8%) 10 13	2, 5, 22, 49	0
1	B	964/989 (97%)	0.38	74 (7%) 13 18	2, 6, 22, 44	0
All	All	1925/1978 (97%)	0.40	159 (8%) 11 14	2, 5, 22, 49	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	VAL	13.5
1	A	152	VAL	11.5
1	B	149	GLY	11.4
1	B	153	THR	11.1
1	A	149	GLY	9.4
1	A	151	ALA	9.4
1	B	151	ALA	9.0
1	B	150	LYS	8.7
1	B	148	ASN	8.1
1	B	147	LEU	8.0
1	A	150	LYS	7.7
1	B	154	THR	7.6
1	B	155	GLU	6.8
1	B	364	SER	6.7
1	B	584	GLU	6.3
1	A	148	ASN	6.0
1	B	377	ASP	6.0
1	A	890	THR	5.9
1	A	971	GLY	5.6
1	B	156	ASP	5.3
1	A	972	ALA	5.2
1	A	153	THR	5.2
1	A	584	GLU	5.2
1	B	157	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	966	ASN	4.8
1	B	572	ASN	4.7
1	A	973	TRP	4.7
1	A	154	THR	4.7
1	B	488[A]	ASN	4.7
1	B	571	PRO	4.6
1	B	890	THR	4.6
1	B	625	SER	4.6
1	B	592	ARG	4.5
1	A	592	ARG	4.4
1	A	572	ASN	4.4
1	B	103	ASN	4.4
1	A	571	PRO	4.3
1	A	941	PRO	4.1
1	A	939	GLY	4.1
1	A	363	GLY	4.0
1	B	145	THR	3.9
1	A	204	LEU	3.9
1	A	940	GLU	3.8
1	A	147	LEU	3.8
1	A	575	THR	3.8
1	A	938	THR	3.7
1	B	489	ASN	3.7
1	A	574	ILE	3.7
1	B	487	ALA	3.7
1	B	363	GLY	3.6
1	A	585	ASP	3.6
1	A	292	LEU	3.5
1	B	375	SER	3.5
1	A	637	LYS	3.5
1	B	146	LYS	3.4
1	A	155	GLU	3.4
1	B	158	THR	3.4
1	B	573	THR	3.4
1	A	666	GLU	3.3
1	A	624	ASN	3.3
1	A	103	ASN	3.2
1	B	117[A]	MET	3.2
1	B	637	LYS	3.1
1	B	374	SER	3.1
1	A	625	SER	3.0
1	A	570	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	585	ASP	3.0
1	B	298	GLU	3.0
1	B	624	ASN	3.0
1	B	362	ASN	3.0
1	A	293	PHE	3.0
1	B	216	ASP	2.9
1	A	687	LEU	2.9
1	A	623	LYS	2.9
1	A	989	PRO	2.8
1	B	614	GLY	2.8
1	A	174	VAL	2.8
1	B	255	ASN	2.8
1	A	667	GLY	2.8
1	B	943	LYS	2.8
1	A	89	LEU	2.8
1	A	452	LEU	2.8
1	B	957	ASN	2.8
1	A	958	ASN	2.7
1	A	322	TRP	2.7
1	B	570	ASP	2.7
1	A	573	THR	2.7
1	B	160	LYS	2.7
1	A	304	PHE	2.7
1	A	291	PRO	2.7
1	A	595	ASP	2.7
1	A	377	ASP	2.6
1	B	627	GLU	2.6
1	B	687	LEU	2.6
1	B	490	LYS	2.6
1	A	157	GLN	2.5
1	A	974	LYS	2.5
1	A	156	ASP	2.5
1	A	474	VAL	2.5
1	A	472	LEU	2.5
1	A	86[A]	ILE	2.5
1	B	810	ASP	2.4
1	B	958	ASN	2.4
1	A	80	VAL	2.4
1	B	144	PRO	2.4
1	A	177	VAL	2.4
1	B	575	THR	2.4
1	B	188	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	366[A]	SER	2.4
1	A	70	ASN	2.4
1	B	378	THR	2.4
1	A	614	GLY	2.3
1	B	104	GLY	2.3
1	B	105	VAL	2.3
1	B	968	VAL	2.3
1	B	986	LEU	2.3
1	A	887	ASN	2.3
1	A	244	ALA	2.3
1	B	705	LEU	2.3
1	B	783[A]	ILE	2.3
1	B	939	GLY	2.3
1	A	688	LEU	2.2
1	B	595	ASP	2.2
1	A	79	VAL	2.2
1	A	630	GLU	2.2
1	A	77	PHE	2.2
1	A	479	VAL	2.2
1	B	101	VAL	2.2
1	A	554	THR	2.2
1	B	215	GLY	2.2
1	B	588	TYR	2.2
1	A	117[A]	MET	2.2
1	A	202	VAL	2.2
1	A	957	ASN	2.2
1	B	960[A]	ASN	2.2
1	A	290	SER	2.1
1	A	760[A]	LEU	2.1
1	B	981	ASN	2.1
1	B	253	GLU	2.1
1	B	376	GLN	2.1
1	A	453	ALA	2.1
1	B	189	ALA	2.1
1	B	217	ASN	2.1
1	A	180	ILE	2.1
1	A	243	ILE	2.1
1	A	590	PHE	2.1
1	A	891	THR	2.1
1	B	354	THR	2.1
1	A	283	ALA	2.1
1	B	941	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	262	ASN	2.1
1	A	638[A]	THR	2.1
1	A	499	ILE	2.1
1	A	264	LYS	2.0
1	B	264	LYS	2.0
1	A	110	PHE	2.0
1	A	203	ARG	2.0
1	A	975	TYR	2.0
1	A	95	VAL	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACT	A	1900	4/4	0.70	0.20	37,38,38,38	0
2	ACT	B	1900	4/4	0.77	0.24	46,47,47,47	0
3	MLA	A	2000	7/7	0.83	0.23	38,41,49,51	0
3	MLA	B	2000	7/7	0.85	0.15	28,34,44,45	0
3	MLA	B	1800	7/7	0.87	0.23	33,37,43,46	0
3	MLA	A	2200	7/7	0.88	0.18	19,22,35,37	0
3	MLA	A	2100	7/7	0.90	0.14	19,22,27,27	0
2	ACT	B	1700	4/4	0.92	0.24	15,15,17,17	0
4	NA	B	2100	1/1	0.92	0.09	28,28,28,28	0
2	ACT	A	1800	4/4	0.93	0.23	14,14,15,15	0
4	NA	B	2300	1/1	0.97	0.10	25,25,25,25	0
4	NA	B	2200	1/1	0.98	0.09	30,30,30,30	0
4	NA	A	2300	1/1	0.98	0.09	20,20,20,20	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.