



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:55 PM UTC

PDB ID : 3A6D / pdb_00003a6d
Title : Creatininase complexed with 1-methylguanidine
Authors : Nakajima, Y.; Yamashita, K.; Ito, K.; Yoshimoto, T.
Deposited on : 2009-08-31
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

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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

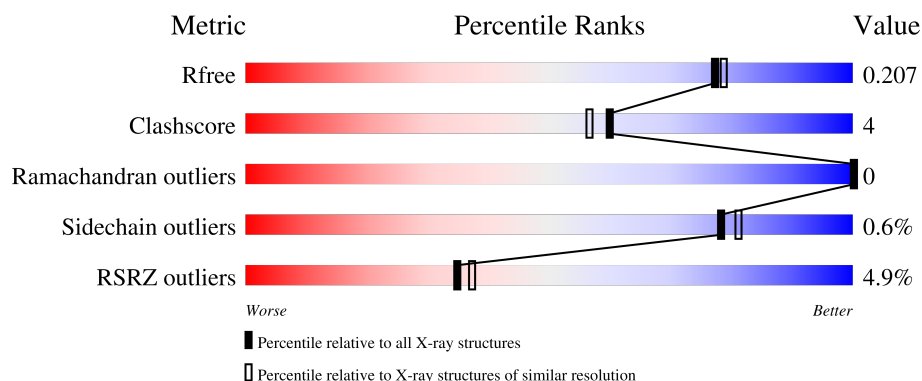
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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 $\leq 5\%$. 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	260	5% 87% 12% .
1	B	260	3% 87% 12% .
1	C	260	5% 86% 12% .
1	D	260	8% 84% 15% .
1	E	260	4% 83% 15% .

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Mol	Chain	Length	Quality of chain
1	F	260	4% 90% 8% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13111 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 Creatinine amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1984	1270	336	367	11			
1	B	256	Total	C	N	O	S	0	0	0
			1976	1264	335	366	11			
1	C	256	Total	C	N	O	S	0	0	0
			1975	1264	334	366	11			
1	D	257	Total	C	N	O	S	0	0	0
			1988	1273	337	367	11			
1	E	257	Total	C	N	O	S	0	0	0
			1984	1270	336	367	11			
1	F	257	Total	C	N	O	S	0	0	0
			1984	1270	336	367	11			

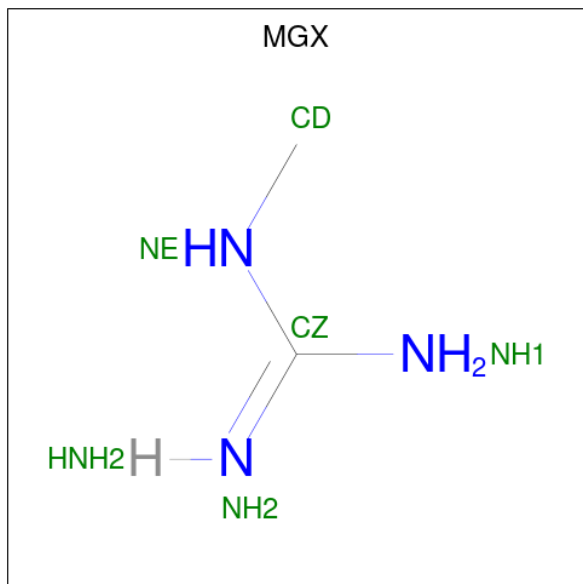
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

- Molecule 4 is 1-METHYLGUANIDINE (CCD ID: MGX) (formula: C₂H₇N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 5 2 3	0	0
4	B	1	Total C N 5 2 3	0	0
4	C	1	Total C N 5 2 3	0	0
4	D	1	Total C N 5 2 3	0	0
4	E	1	Total C N 5 2 3	0	0
4	F	1	Total C N 5 2 3	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

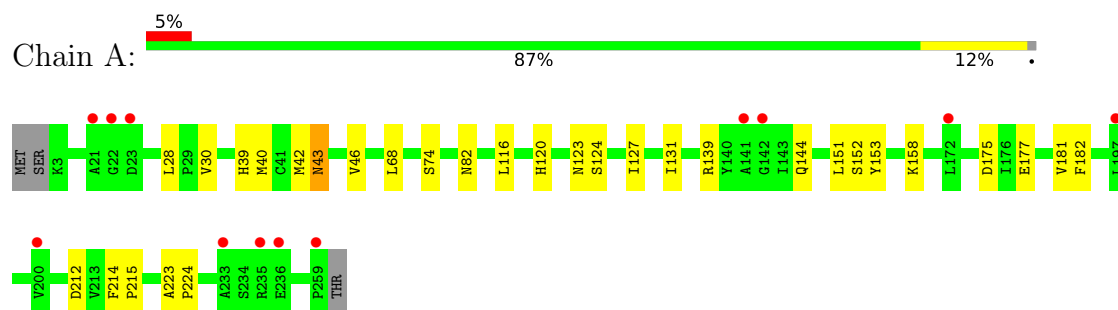
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	183	Total	O	0	0
			183	183		
6	B	186	Total	O	0	0
			186	186		
6	C	189	Total	O	0	0
			189	189		
6	D	160	Total	O	0	0
			160	160		
6	E	186	Total	O	0	0
			186	186		
6	F	184	Total	O	0	0
			184	184		

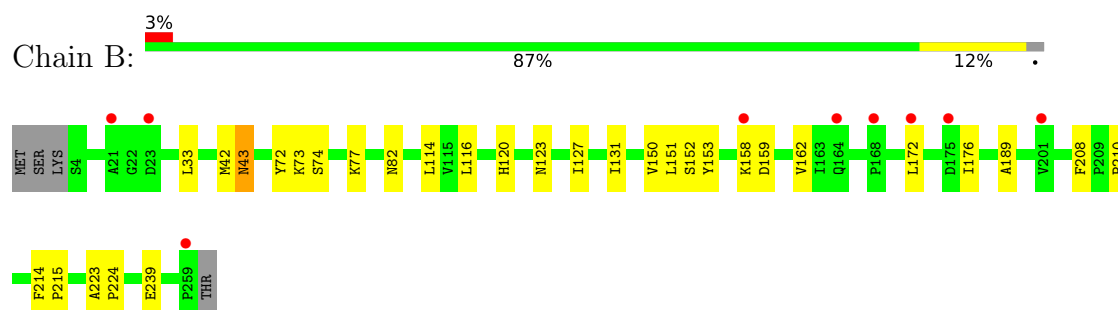
3 Residue-property plots [i](#)

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.

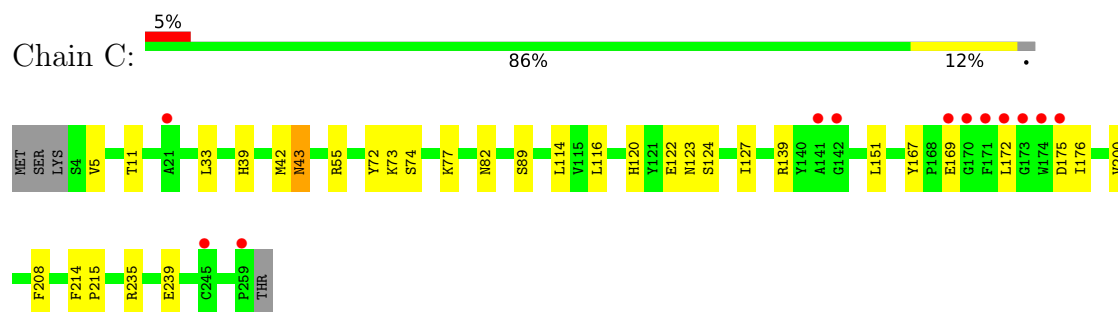
- Molecule 1: Creatinine amidohydrolase



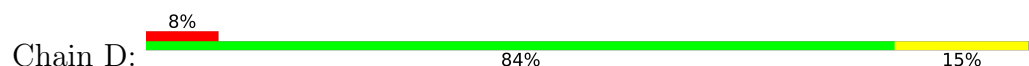
- Molecule 1: Creatinine amidohydrolase

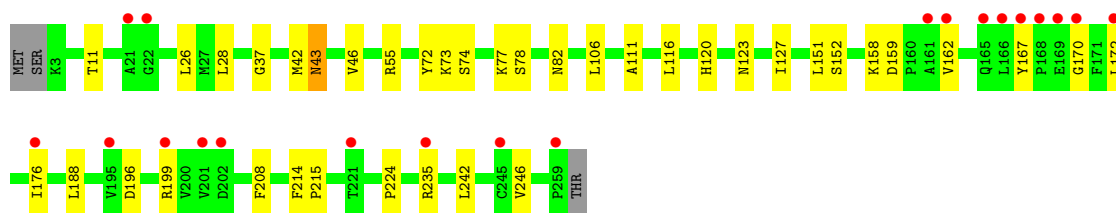


- Molecule 1: Creatinine amidohydrolase

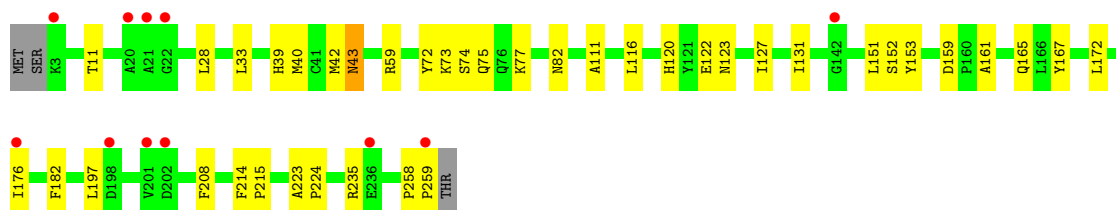
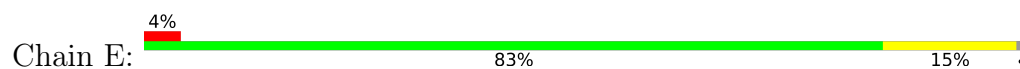


- Molecule 1: Creatinine amidohydrolase

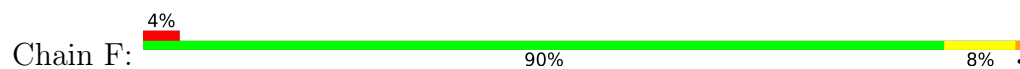




● Molecule 1: Creatinine amidohydrolase



● Molecule 1: Creatinine amidohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.40Å 152.70Å 167.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-1.90) 98.6 (20.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.207 0.193 , 0.207	Depositor DCC
R_{free} test set	10246 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13111	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, MN, SO4, MGX

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	0.36	0/2033	0.88	7/2768 (0.3%)
1	B	0.36	0/2025	0.89	5/2757 (0.2%)
1	C	0.36	0/2024	0.90	7/2757 (0.3%)
1	D	0.36	0/2037	0.88	6/2772 (0.2%)
1	E	0.35	0/2033	0.88	7/2768 (0.3%)
1	F	0.36	0/2033	0.88	6/2768 (0.2%)
All	All	0.36	0/12185	0.88	38/16590 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	ILE	N-CA-C	-6.54	104.12	110.72
1	B	127	ILE	N-CA-C	-6.21	104.69	110.53
1	F	127	ILE	N-CA-C	-6.19	104.47	110.72
1	A	127	ILE	N-CA-C	-6.04	104.61	110.72
1	B	152	SER	N-CA-C	-6.00	98.73	108.52
1	E	127	ILE	N-CA-C	-5.99	104.67	110.72
1	F	152	SER	N-CA-C	-5.89	98.93	108.52
1	A	152	SER	N-CA-C	-5.84	99.00	108.52
1	E	152	SER	N-CA-C	-5.82	99.03	108.52
1	D	127	ILE	N-CA-C	-5.78	104.88	110.72
1	D	152	SER	N-CA-C	-5.74	99.17	108.52
1	F	42	MET	N-CA-C	5.71	120.24	113.16
1	C	42	MET	N-CA-C	5.69	120.38	113.38
1	F	33	LEU	N-CA-C	-5.67	97.95	107.99
1	B	153	TYR	N-CA-C	5.57	118.88	111.75
1	C	89	SER	N-CA-C	5.57	118.80	109.95
1	D	11	THR	N-CA-C	-5.55	102.30	110.52
1	A	153	TYR	N-CA-C	5.54	118.85	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	LEU	N-CA-C	-5.48	98.44	108.02
1	D	46	VAL	N-CA-C	-5.45	106.49	111.67
1	B	42	MET	N-CA-C	5.42	119.88	113.16
1	D	42	MET	N-CA-C	5.35	119.80	113.28
1	C	124	SER	N-CA-C	5.30	122.09	110.80
1	E	153	TYR	N-CA-C	5.29	118.52	111.75
1	A	124	SER	N-CA-C	5.28	122.05	110.80
1	C	11	THR	N-CA-C	-5.25	102.75	110.52
1	A	42	MET	N-CA-C	5.24	119.78	113.17
1	A	46	VAL	N-CA-C	-5.22	106.71	111.67
1	C	33	LEU	N-CA-C	-5.22	98.75	107.99
1	D	158	LYS	CB-CA-C	-5.20	100.29	109.02
1	A	181	VAL	N-CA-C	5.19	115.41	110.42
1	E	33	LEU	N-CA-C	-5.18	98.81	107.99
1	E	11	THR	N-CA-C	-5.17	102.88	110.52
1	E	42	MET	N-CA-C	5.16	119.67	113.17
1	E	59	ARG	N-CA-C	5.14	116.96	111.36
1	C	122	GLU	N-CA-C	5.05	118.54	112.38
1	F	11	THR	N-CA-C	-5.03	103.07	110.52
1	F	91	ASP	N-CA-C	-5.00	103.80	110.55

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	1984	0	1958	17	0
1	B	1976	0	1947	15	0
1	C	1975	0	1945	18	0
1	D	1988	0	1969	21	0
1	E	1984	0	1958	22	0
1	F	1984	0	1958	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	6	0	0
4	B	5	0	6	0	0
4	C	5	0	6	0	0
4	D	5	0	6	1	0
4	E	5	0	6	0	0
4	F	5	0	6	0	0
5	A	15	0	0	0	0
5	B	15	0	0	0	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
5	E	15	0	0	0	0
5	F	15	0	0	0	0
6	A	183	0	0	0	0
6	B	186	0	0	0	0
6	C	189	0	0	1	0
6	D	160	0	0	1	0
6	E	186	0	0	1	0
6	F	184	0	0	0	0
All	All	13111	0	11771	103	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 4.

All (103) 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:E:172:LEU:HB3	1:E:176:ILE:HD11	1.29	1.11
1:D:172:LEU:HB3	1:D:176:ILE:HD11	1.48	0.95
1:A:116:LEU:HD12	1:A:131:ILE:HD11	1.75	0.68
1:E:161:ALA:O	1:E:165:GLN:HG3	1.96	0.65
1:E:120:HIS:HB3	1:E:123:ASN:ND2	2.12	0.65
1:A:139:ARG:HH12	1:A:144:GLN:NE2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:SER:H	1:C:82:ASN:HD22	1.44	0.64
1:E:172:LEU:HB3	1:E:176:ILE:CD1	2.18	0.64
1:A:139:ARG:HH12	1:A:144:GLN:CD	2.09	0.60
1:F:172:LEU:HB2	1:F:176:ILE:HD11	1.83	0.60
1:F:120:HIS:HB3	1:F:123:ASN:ND2	2.18	0.59
1:D:74:SER:H	1:D:82:ASN:HD22	1.52	0.58
1:A:139:ARG:NH1	1:A:144:GLN:CD	2.61	0.58
1:B:120:HIS:HB3	1:B:123:ASN:ND2	2.20	0.57
1:F:235:ARG:O	1:F:239:GLU:HG3	2.05	0.57
1:D:120:HIS:HB3	1:D:123:ASN:ND2	2.20	0.56
1:D:196:ASP:HB3	1:D:199:ARG:HD2	1.88	0.56
1:D:214:PHE:HA	1:D:215:PRO:C	2.31	0.56
1:F:214:PHE:HA	1:F:215:PRO:C	2.30	0.56
1:C:43:ASN:C	1:C:43:ASN:HD22	2.15	0.55
1:E:74:SER:H	1:E:82:ASN:HD22	1.54	0.54
1:E:214:PHE:HA	1:E:215:PRO:C	2.32	0.54
1:C:214:PHE:HA	1:C:215:PRO:C	2.33	0.53
1:F:116:LEU:HD22	1:F:127:ILE:HG23	1.90	0.53
1:A:139:ARG:NH1	1:A:144:GLN:NE2	2.56	0.53
1:D:188:LEU:O	1:D:235:ARG:NH2	2.42	0.53
1:F:74:SER:H	1:F:82:ASN:HD22	1.55	0.53
1:A:120:HIS:HB3	1:A:123:ASN:ND2	2.24	0.52
1:B:214:PHE:HA	1:B:215:PRO:C	2.34	0.52
1:C:235:ARG:O	1:C:239:GLU:HG3	2.10	0.52
1:C:120:HIS:HB3	1:C:123:ASN:ND2	2.24	0.52
1:D:28:LEU:HD23	1:D:116:LEU:HD21	1.92	0.52
1:A:74:SER:H	1:A:82:ASN:HD22	1.58	0.52
1:D:77:LYS:HE2	1:D:208:PHE:CB	2.41	0.51
1:B:114:LEU:HD21	1:B:116:LEU:HD11	1.93	0.50
1:A:214:PHE:HA	1:A:215:PRO:C	2.35	0.50
1:D:167:TYR:HB3	1:D:170:GLY:O	2.11	0.50
1:E:39:HIS:CD2	1:E:40:MET:HG3	2.47	0.50
1:B:43:ASN:C	1:B:43:ASN:HD22	2.19	0.49
1:F:43:ASN:C	1:F:43:ASN:HD22	2.20	0.49
1:F:169:GLU:HG2	1:F:169:GLU:O	2.13	0.49
1:E:43:ASN:HD22	1:E:43:ASN:C	2.20	0.49
1:D:242:LEU:O	1:D:246:VAL:HG23	2.13	0.48
1:A:43:ASN:HD22	1:A:43:ASN:C	2.22	0.48
1:A:151:LEU:C	1:A:151:LEU:HD12	2.39	0.48
1:C:172:LEU:HB2	1:C:176:ILE:HD11	1.95	0.48
1:F:223:ALA:HB3	1:F:224:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:TYR:OH	1:E:182:PHE:HB2	2.13	0.48
1:C:114:LEU:HG	1:C:116:LEU:HD12	1.96	0.47
1:D:28:LEU:HD23	1:D:116:LEU:CD2	2.44	0.47
1:D:151:LEU:HD12	1:D:151:LEU:C	2.39	0.47
1:E:116:LEU:HD12	1:E:131:ILE:HD11	1.95	0.47
1:B:77:LYS:HE2	1:B:208:PHE:HB2	1.95	0.47
1:E:75:GLN:HG2	1:E:122:GLU:HG2	1.97	0.47
1:E:159:ASP:OD2	1:E:161:ALA:HB3	2.15	0.47
1:D:43:ASN:HD22	1:D:43:ASN:C	2.22	0.46
1:A:158:LYS:HD3	1:B:210:PRO:HG3	1.97	0.45
1:E:77:LYS:HE2	1:E:208:PHE:CB	2.46	0.45
1:B:131:ILE:CD1	1:B:150:VAL:HG21	2.47	0.45
1:A:30:VAL:HG13	1:A:68:LEU:HD12	1.99	0.45
1:D:111:ALA:HB1	6:D:1986:HOH:O	2.16	0.45
1:E:28:LEU:HD23	1:E:116:LEU:CD2	2.46	0.45
1:B:159:ASP:OD2	1:B:162:VAL:HG23	2.17	0.45
1:B:151:LEU:C	1:B:151:LEU:HD12	2.42	0.44
1:B:74:SER:H	1:B:82:ASN:HD22	1.64	0.44
1:D:159:ASP:OD2	1:D:162:VAL:HG23	2.17	0.44
1:E:235:ARG:HB2	1:E:235:ARG:HH21	1.83	0.44
1:C:151:LEU:HD12	1:C:151:LEU:C	2.42	0.43
1:A:223:ALA:HB3	1:A:224:PRO:HD3	1.99	0.43
1:D:26:LEU:CD1	1:D:106:LEU:HD22	2.48	0.43
1:C:114:LEU:HD21	1:C:116:LEU:HD11	2.00	0.43
1:C:167:TYR:C	1:C:169:GLU:H	2.26	0.43
1:B:172:LEU:CB	1:B:176:ILE:HD11	2.49	0.43
1:D:77:LYS:HE2	1:D:208:PHE:HB2	2.00	0.43
1:A:39:HIS:CD2	1:A:40:MET:HG3	2.54	0.43
1:C:77:LYS:HE2	1:C:208:PHE:HB2	2.01	0.43
1:D:78:SER:O	4:D:305:MGX:NH2	2.52	0.43
1:E:111:ALA:HB1	6:E:1957:HOH:O	2.18	0.43
1:A:139:ARG:HH11	1:A:139:ARG:HG3	1.84	0.42
1:E:258:PRO:HA	1:E:259:PRO:HD3	1.89	0.42
1:D:37:GLY:HA2	1:D:224:PRO:O	2.19	0.42
1:C:43:ASN:C	1:C:43:ASN:ND2	2.77	0.42
1:D:55:ARG:HG3	1:D:55:ARG:HH11	1.84	0.42
1:E:223:ALA:HB3	1:E:224:PRO:HD3	2.00	0.42
1:C:72:TYR:CG	1:C:73:LYS:N	2.87	0.42
1:C:175:ASP:OD2	1:C:175:ASP:N	2.53	0.42
1:D:72:TYR:CG	1:D:73:LYS:N	2.88	0.42
1:A:28:LEU:HB3	1:A:116:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ARG:HH11	1:C:55:ARG:HG3	1.84	0.42
1:F:175:ASP:OD2	1:F:176:ILE:N	2.53	0.41
1:C:139:ARG:HB2	1:C:139:ARG:NH1	2.36	0.41
1:E:72:TYR:CG	1:E:73:LYS:N	2.89	0.41
1:E:151:LEU:C	1:E:151:LEU:HD12	2.46	0.41
1:A:177:GLU:HG3	1:A:182:PHE:HB3	2.02	0.41
1:B:158:LYS:HE3	1:B:158:LYS:HB2	1.90	0.40
1:B:223:ALA:HB3	1:B:224:PRO:HD3	2.03	0.40
1:E:197:LEU:HD12	1:E:197:LEU:HA	1.95	0.40
1:E:116:LEU:CD1	1:E:131:ILE:HD11	2.52	0.40
1:C:39:HIS:CG	1:C:200:VAL:HG22	2.56	0.40
1:F:75:GLN:HG2	1:F:122:GLU:HG2	2.03	0.40
1:B:189:ALA:HB1	1:B:239:GLU:OE2	2.22	0.40
1:C:5:VAL:HG22	6:C:1302:HOH:O	2.21	0.40
1:B:72:TYR:CG	1:B:73:LYS:N	2.89	0.40

There are no symmetry-related clashes.

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	255/260 (98%)	248 (97%)	7 (3%)	0	100	100
1	B	254/260 (98%)	247 (97%)	7 (3%)	0	100	100
1	C	254/260 (98%)	247 (97%)	7 (3%)	0	100	100
1	D	255/260 (98%)	249 (98%)	6 (2%)	0	100	100
1	E	255/260 (98%)	249 (98%)	6 (2%)	0	100	100
1	F	255/260 (98%)	249 (98%)	6 (2%)	0	100	100
All	All	1528/1560 (98%)	1489 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	211/215 (98%)	208 (99%)	3 (1%)	59	59
1	B	210/215 (98%)	209 (100%)	1 (0%)	81	84
1	C	210/215 (98%)	209 (100%)	1 (0%)	81	84
1	D	212/215 (99%)	211 (100%)	1 (0%)	81	84
1	E	211/215 (98%)	210 (100%)	1 (0%)	81	84
1	F	211/215 (98%)	210 (100%)	1 (0%)	81	84
All	All	1265/1290 (98%)	1257 (99%)	8 (1%)	78	81

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	175	ASP
1	A	212	ASP
1	B	43	ASN
1	C	43	ASN
1	D	43	ASN
1	E	43	ASN
1	F	43	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	76	GLN
1	A	82	ASN
1	A	118	ASN
1	A	144	GLN
1	B	43	ASN
1	B	82	ASN
1	B	118	ASN
1	B	165	GLN

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Mol	Chain	Res	Type
1	C	43	ASN
1	C	76	GLN
1	C	82	ASN
1	C	118	ASN
1	D	43	ASN
1	D	69	GLN
1	D	82	ASN
1	D	118	ASN
1	D	144	GLN
1	D	165	GLN
1	E	43	ASN
1	E	76	GLN
1	E	82	ASN
1	E	118	ASN
1	E	165	GLN
1	F	43	ASN
1	F	76	GLN
1	F	82	ASN
1	F	118	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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
5	SO4	C	418	-	4,4,4	0.39	0	6,6,6	0.12	0
4	MGX	A	302	-	4,4,4	3.28	1 (25%)	4,4,4	1.17	0
5	SO4	C	412	-	4,4,4	0.38	0	6,6,6	0.06	0
4	MGX	F	307	-	4,4,4	3.35	1 (25%)	4,4,4	1.16	0
5	SO4	A	404	-	4,4,4	0.39	0	6,6,6	0.07	0
5	SO4	F	403	-	4,4,4	0.39	0	6,6,6	0.10	0
4	MGX	B	303	-	4,4,4	3.32	1 (25%)	4,4,4	1.15	0
5	SO4	D	407	-	4,4,4	0.41	0	6,6,6	0.09	0
5	SO4	E	408	-	4,4,4	0.41	0	6,6,6	0.06	0
5	SO4	D	401	-	4,4,4	0.38	0	6,6,6	0.09	0
5	SO4	A	410	-	4,4,4	0.35	0	6,6,6	0.08	0
4	MGX	C	304	-	4,4,4	3.34	1 (25%)	4,4,4	1.20	0
5	SO4	A	416	-	4,4,4	0.36	0	6,6,6	0.09	0
5	SO4	B	405	-	4,4,4	0.40	0	6,6,6	0.08	0
5	SO4	E	414	-	4,4,4	0.37	0	6,6,6	0.06	0
5	SO4	D	413	-	4,4,4	0.36	0	6,6,6	0.09	0
5	SO4	E	402	-	4,4,4	0.38	0	6,6,6	0.10	0
5	SO4	C	406	-	4,4,4	0.41	0	6,6,6	0.06	0
4	MGX	E	306	-	4,4,4	3.35	1 (25%)	4,4,4	1.36	0
5	SO4	F	409	-	4,4,4	0.39	0	6,6,6	0.06	0
5	SO4	F	415	-	4,4,4	0.36	0	6,6,6	0.09	0
5	SO4	B	411	-	4,4,4	0.38	0	6,6,6	0.05	0
5	SO4	B	417	-	4,4,4	0.40	0	6,6,6	0.09	0
4	MGX	D	305	-	4,4,4	3.22	1 (25%)	4,4,4	1.27	0

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	MGX	B	303	-	-	0/2/2/2	-
4	MGX	A	302	-	-	0/2/2/2	-
4	MGX	F	307	-	-	0/2/2/2	-
4	MGX	E	306	-	-	0/2/2/2	-
4	MGX	C	304	-	-	0/2/2/2	-
4	MGX	D	305	-	-	0/2/2/2	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	307	MGX	CD-NE	-6.58	1.33	1.45
4	C	304	MGX	CD-NE	-6.54	1.34	1.45
4	E	306	MGX	CD-NE	-6.53	1.34	1.45
4	B	303	MGX	CD-NE	-6.51	1.34	1.45
4	A	302	MGX	CD-NE	-6.42	1.34	1.45
4	D	305	MGX	CD-NE	-6.30	1.34	1.45

There are no bond angle outliers.

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
4	D	305	MGX	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, 95th 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 ²)	Q<0.9
1	A	257/260 (98%)	0.15	12 (4%) 36 39	18, 27, 42, 49	0
1	B	256/260 (98%)	0.07	9 (3%) 47 50	18, 28, 45, 52	0
1	C	256/260 (98%)	0.09	12 (4%) 36 39	18, 27, 43, 53	0
1	D	257/260 (98%)	0.38	20 (7%) 19 20	19, 30, 45, 51	0
1	E	257/260 (98%)	0.16	11 (4%) 40 42	19, 28, 42, 48	0
1	F	257/260 (98%)	0.02	11 (4%) 40 42	17, 27, 44, 55	0
All	All	1540/1560 (98%)	0.15	75 (4%) 35 37	17, 28, 44, 55	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	ALA	5.2
1	C	174	TRP	5.1
1	A	21	ALA	4.9
1	F	169	GLU	4.7
1	C	175	ASP	4.4
1	F	172	LEU	4.4
1	D	167	TYR	4.4
1	B	259	PRO	4.3
1	F	175	ASP	4.2
1	D	166	LEU	4.2
1	D	259	PRO	4.1
1	C	172	LEU	4.0
1	E	21	ALA	4.0
1	D	162	VAL	3.8
1	F	171	PHE	3.8
1	C	173	GLY	3.6
1	A	172	LEU	3.6
1	C	171	PHE	3.6
1	A	259	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	174	TRP	3.4
1	E	176	ILE	3.4
1	B	21	ALA	3.3
1	C	169	GLU	3.2
1	D	21	ALA	3.2
1	D	165	GLN	3.2
1	B	164	GLN	3.2
1	A	236	GLU	3.2
1	D	161	ALA	3.1
1	E	259	PRO	3.1
1	C	259	PRO	3.0
1	D	235	ARG	3.0
1	D	22	GLY	3.0
1	A	142	GLY	3.0
1	A	197	LEU	2.9
1	A	200	VAL	2.9
1	B	201	VAL	2.9
1	D	168	PRO	2.9
1	B	172	LEU	2.9
1	A	22	GLY	2.8
1	A	141	ALA	2.8
1	E	201	VAL	2.7
1	D	176	ILE	2.7
1	F	173	GLY	2.7
1	B	175	ASP	2.6
1	D	172	LEU	2.6
1	D	202	ASP	2.6
1	E	236	GLU	2.6
1	A	23	ASP	2.5
1	D	195	VAL	2.5
1	F	259	PRO	2.5
1	F	170	GLY	2.5
1	C	142	GLY	2.4
1	C	141	ALA	2.4
1	C	245	CYS	2.4
1	A	235	ARG	2.3
1	C	170	GLY	2.3
1	E	22	GLY	2.3
1	B	168	PRO	2.3
1	F	22	GLY	2.3
1	D	169	GLU	2.3
1	D	245	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	3	LYS	2.3
1	D	201	VAL	2.3
1	D	199	ARG	2.2
1	E	202	ASP	2.2
1	B	158	LYS	2.2
1	B	23	ASP	2.2
1	F	21	ALA	2.2
1	F	139	ARG	2.2
1	A	233	ALA	2.2
1	D	170	GLY	2.1
1	E	198	ASP	2.1
1	E	20	ALA	2.1
1	D	221	THR	2.0
1	E	142	GLY	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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
4	MGX	E	306	5/5	0.74	0.28	42,45,46,49	0
5	SO4	D	407	5/5	0.74	0.15	66,66,67,68	0
5	SO4	B	405	5/5	0.75	0.16	71,71,72,74	0
4	MGX	D	305	5/5	0.77	0.34	45,48,49,49	0
5	SO4	F	409	5/5	0.78	0.14	70,70,71,72	0
4	MGX	C	304	5/5	0.80	0.22	43,43,45,45	0
4	MGX	A	302	5/5	0.82	0.17	30,33,35,35	0
5	SO4	F	403	5/5	0.83	0.11	65,65,66,67	0
5	SO4	E	402	5/5	0.83	0.10	63,63,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	C	418	5/5	0.84	0.11	63,64,65,66	0
5	SO4	D	401	5/5	0.84	0.11	58,58,59,60	0
5	SO4	E	408	5/5	0.85	0.12	66,66,67,68	0
4	MGX	F	307	5/5	0.86	0.17	41,42,43,43	0
5	SO4	C	406	5/5	0.87	0.10	65,66,66,68	0
5	SO4	B	417	5/5	0.88	0.09	63,63,65,65	0
5	SO4	A	404	5/5	0.89	0.10	64,65,65,66	0
4	MGX	B	303	5/5	0.90	0.12	35,36,36,37	0
5	SO4	A	416	5/5	0.90	0.12	59,60,61,62	0
5	SO4	D	413	5/5	0.95	0.07	45,45,47,48	0
5	SO4	C	412	5/5	0.96	0.09	36,39,40,40	0
5	SO4	E	414	5/5	0.96	0.09	43,43,44,45	0
5	SO4	F	415	5/5	0.96	0.11	39,41,43,43	0
5	SO4	B	411	5/5	0.97	0.07	37,37,39,39	0
5	SO4	A	410	5/5	0.97	0.07	35,35,37,39	0
2	MN	D	300	1/1	0.98	0.03	28,28,28,28	0
2	MN	B	300	1/1	0.99	0.02	23,23,23,23	0
2	MN	A	300	1/1	0.99	0.02	23,23,23,23	0
2	MN	E	300	1/1	0.99	0.02	26,26,26,26	0
3	ZN	A	301	1/1	0.99	0.03	26,26,26,26	0
3	ZN	B	301	1/1	0.99	0.02	26,26,26,26	0
3	ZN	C	301	1/1	0.99	0.02	27,27,27,27	0
3	ZN	D	301	1/1	0.99	0.03	29,29,29,29	0
3	ZN	E	301	1/1	0.99	0.02	27,27,27,27	0
2	MN	F	300	1/1	1.00	0.01	24,24,24,24	0
2	MN	C	300	1/1	1.00	0.01	24,24,24,24	0
3	ZN	F	301	1/1	1.00	0.01	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.