



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:48 AM UTC

PDB ID : 1Q3K / pdb_00001q3k
Title : Crystal structure of creatinine amidohydrolase (creatininase)
Authors : Beuth, B.; Niefind, K.; Schomburg, D.
Deposited on : 2003-07-30
Resolution : 2.10 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

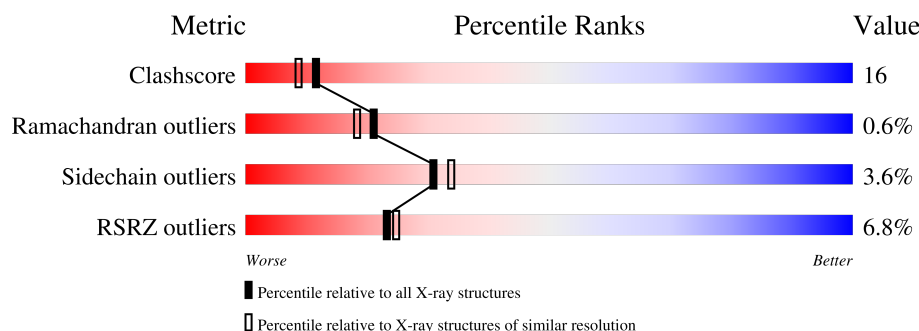
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	259	6% 69% 28% .
1	B	259	5% 69% 27% .
1	C	259	9% 67% 30% .
1	D	259	8% 70% 27% .
1	E	259	6% 73% 25% .
1	F	259	7% 72% 25% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12760 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 creatininase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total 2000	C 1281	N 340	O 369	S 10	0	0	0
1	B	259	Total 2000	C 1281	N 340	O 369	S 10	0	0	0
1	C	259	Total 2000	C 1281	N 340	O 369	S 10	0	0	0
1	D	259	Total 2000	C 1281	N 340	O 369	S 10	0	0	0
1	E	259	Total 2000	C 1281	N 340	O 369	S 10	0	0	0
1	F	259	Total 2000	C 1281	N 340	O 369	S 10	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	GLN	LYS	conflict	UNP P83772
A	65	LEU	MET	conflict	UNP P83772
A	111	VAL	ALA	conflict	UNP P83772
A	144	HIS	GLN	conflict	UNP P83772
A	165	ARG	GLN	conflict	UNP P83772
A	198	GLU	ASP	conflict	UNP P83772
A	254	GLY	ARG	conflict	UNP P83772
A	255	GLN	GLU	conflict	UNP P83772
B	54	GLN	LYS	conflict	UNP P83772
B	65	LEU	MET	conflict	UNP P83772
B	111	VAL	ALA	conflict	UNP P83772
B	144	HIS	GLN	conflict	UNP P83772
B	165	ARG	GLN	conflict	UNP P83772
B	198	GLU	ASP	conflict	UNP P83772
B	254	GLY	ARG	conflict	UNP P83772
B	255	GLN	GLU	conflict	UNP P83772
C	54	GLN	LYS	conflict	UNP P83772

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	65	LEU	MET	conflict	UNP P83772
C	111	VAL	ALA	conflict	UNP P83772
C	144	HIS	GLN	conflict	UNP P83772
C	165	ARG	GLN	conflict	UNP P83772
C	198	GLU	ASP	conflict	UNP P83772
C	254	GLY	ARG	conflict	UNP P83772
C	255	GLN	GLU	conflict	UNP P83772
D	54	GLN	LYS	conflict	UNP P83772
D	65	LEU	MET	conflict	UNP P83772
D	111	VAL	ALA	conflict	UNP P83772
D	144	HIS	GLN	conflict	UNP P83772
D	165	ARG	GLN	conflict	UNP P83772
D	198	GLU	ASP	conflict	UNP P83772
D	254	GLY	ARG	conflict	UNP P83772
D	255	GLN	GLU	conflict	UNP P83772
E	54	GLN	LYS	conflict	UNP P83772
E	65	LEU	MET	conflict	UNP P83772
E	111	VAL	ALA	conflict	UNP P83772
E	144	HIS	GLN	conflict	UNP P83772
E	165	ARG	GLN	conflict	UNP P83772
E	198	GLU	ASP	conflict	UNP P83772
E	254	GLY	ARG	conflict	UNP P83772
E	255	GLN	GLU	conflict	UNP P83772
F	54	GLN	LYS	conflict	UNP P83772
F	65	LEU	MET	conflict	UNP P83772
F	111	VAL	ALA	conflict	UNP P83772
F	144	HIS	GLN	conflict	UNP P83772
F	165	ARG	GLN	conflict	UNP P83772
F	198	GLU	ASP	conflict	UNP P83772
F	254	GLY	ARG	conflict	UNP P83772
F	255	GLN	GLU	conflict	UNP P83772

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

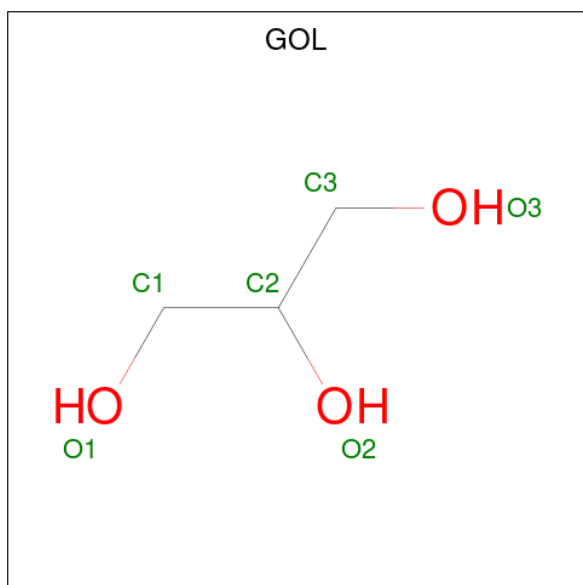
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total	O	0	0
			125	125		
4	B	110	Total	O	0	0
			110	110		
4	C	117	Total	O	0	0
			117	117		

Continued on next page...

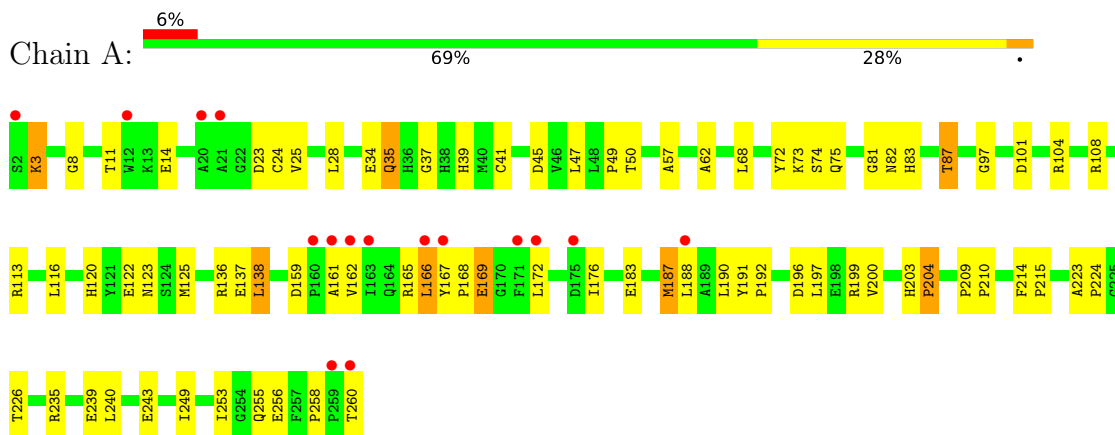
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	113	Total 113	O 113	0	0
4	E	125	Total 125	O 125	0	0
4	F	134	Total 134	O 134	0	0

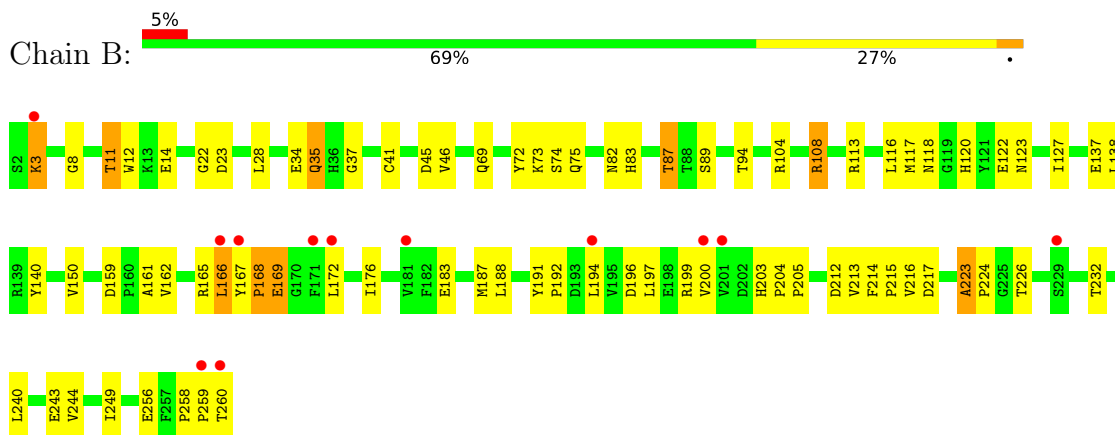
3 Residue-property plots

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 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.

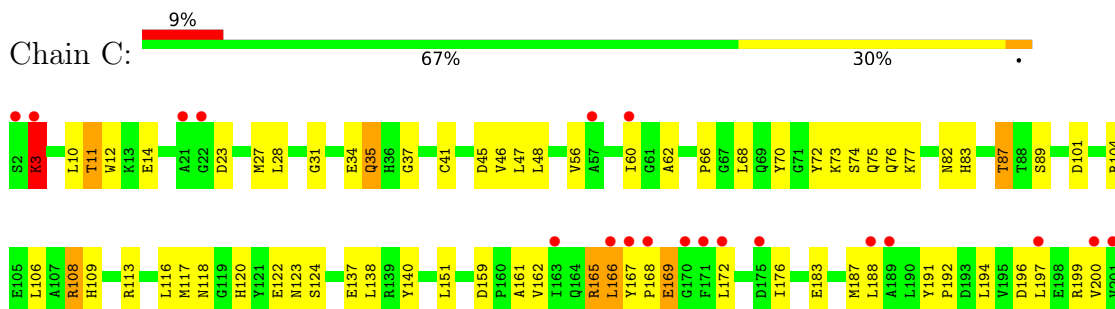
• Molecule 1: creatininase



• Molecule 1: creatininase

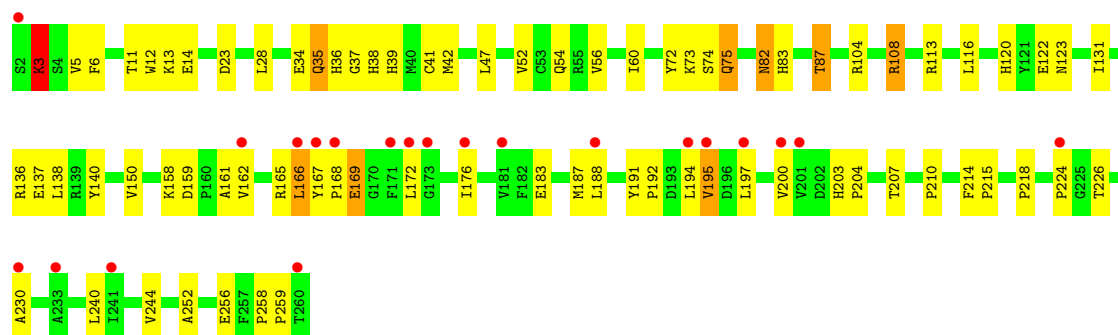


• Molecule 1: creatininase

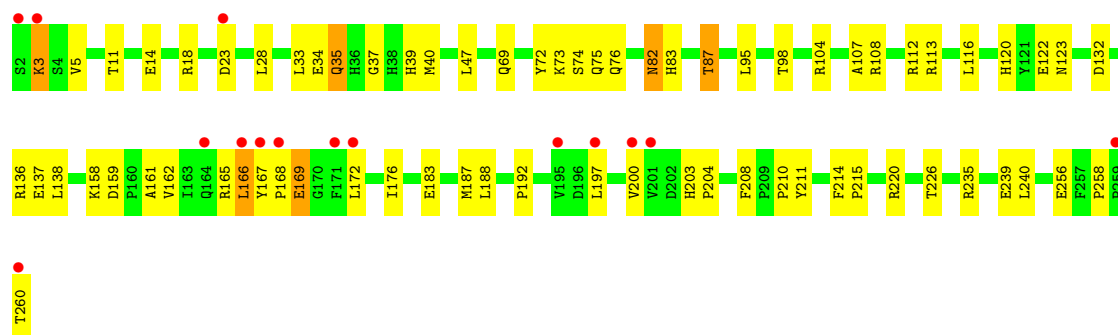
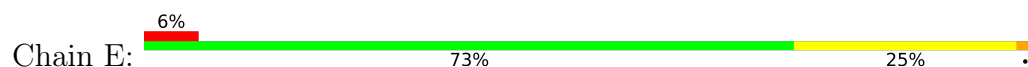




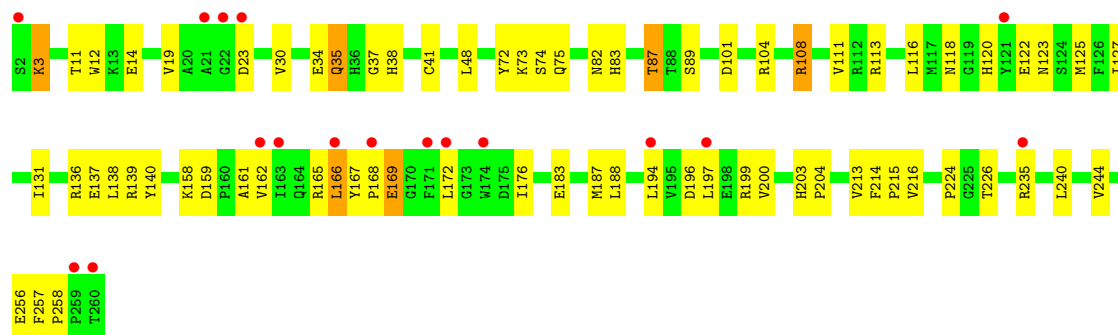
• Molecule 1: creatininase



• Molecule 1: creatininase



• Molecule 1: creatininase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.39Å 94.08Å 114.75Å 90.00° 104.62° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	79.5 (50.00-2.10) 79.5 (50.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.0, CNS	Depositor
R, R_{free}	0.207 , 0.247 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12760	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8434e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.18	5/2050 (0.2%)	1.09	4/2792 (0.1%)
1	B	1.20	3/2050 (0.1%)	1.07	5/2792 (0.2%)
1	C	1.23	3/2050 (0.1%)	1.11	4/2792 (0.1%)
1	D	1.17	2/2050 (0.1%)	1.06	1/2792 (0.0%)
1	E	1.19	5/2050 (0.2%)	1.05	1/2792 (0.0%)
1	F	1.20	2/2050 (0.1%)	1.06	1/2792 (0.0%)
All	All	1.20	20/12300 (0.2%)	1.07	16/16752 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	ASP	C-O	-6.96	1.15	1.24
1	C	204	PRO	C-O	-6.91	1.18	1.24
1	E	112	ARG	C-O	-6.32	1.15	1.24
1	B	94	THR	N-CA	-6.28	1.38	1.46
1	A	24	CYS	CA-C	5.95	1.60	1.52
1	B	108	ARG	C-O	-5.93	1.17	1.24
1	D	75	GLN	C-O	5.84	1.30	1.23
1	E	98	THR	N-CA	-5.77	1.39	1.46
1	A	25	VAL	CA-CB	-5.74	1.47	1.54
1	C	70	TYR	CA-C	-5.57	1.46	1.52
1	E	107	ALA	CA-CB	-5.53	1.44	1.53
1	E	95	LEU	C-O	-5.52	1.17	1.24
1	D	42	MET	CA-C	5.51	1.60	1.52
1	A	125	MET	C-O	-5.46	1.17	1.24
1	C	45	ASP	C-O	-5.38	1.17	1.24
1	A	81	GLY	C-O	-5.24	1.19	1.23
1	F	213	VAL	C-O	-5.22	1.18	1.24
1	A	187	MET	SD-CE	-5.12	1.66	1.79
1	E	132	ASP	C-O	-5.08	1.18	1.24
1	F	125	MET	SD-CE	-5.00	1.67	1.79

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	204	PRO	O-C-N	6.34	124.13	121.15
1	D	39	HIS	N-CA-C	6.01	120.77	113.38
1	B	223	ALA	CA-C-O	5.89	123.75	118.33
1	C	11	THR	N-CA-C	-5.83	102.13	110.59
1	A	39	HIS	N-CA-C	5.76	120.47	113.38
1	C	124	SER	N-CA-C	5.66	122.85	110.80
1	B	11	THR	N-CA-C	-5.44	102.70	110.59
1	C	46	VAL	N-CA-C	-5.38	106.56	111.67
1	A	97	GLY	CA-C-N	5.25	127.27	120.44
1	A	97	GLY	C-N-CA	5.25	127.27	120.44
1	A	204	PRO	O-C-N	5.14	123.57	121.15
1	B	127	ILE	N-CA-C	-5.14	105.53	110.72
1	B	89	SER	N-CA-C	5.13	118.10	109.95
1	B	150	VAL	CB-CA-C	-5.11	103.04	110.81
1	C	31	GLY	N-CA-C	5.03	118.77	110.77
1	E	33	LEU	N-CA-C	-5.02	99.10	107.99

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	2000	0	1980	69	0
1	B	2000	0	1980	66	0
1	C	2000	0	1980	74	0
1	D	2000	0	1980	73	0
1	E	2000	0	1980	56	0
1	F	2000	0	1980	62	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	8	1	0
3	B	6	0	8	2	0
3	C	6	0	8	1	0
3	E	6	0	8	1	0
4	A	125	0	0	13	0
4	B	110	0	0	10	0
4	C	117	0	0	11	0
4	D	113	0	0	15	1
4	E	125	0	0	9	0
4	F	134	0	0	11	1
All	All	12760	0	11912	382	1

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 (382) 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:136:ARG:HD3	4:E:962:HOH:O	1.59	1.02
1:E:3:LYS:HZ2	1:E:3:LYS:HA	1.24	1.00
1:A:3:LYS:HZ2	1:A:3:LYS:HA	1.25	0.99
1:E:3:LYS:HA	1:E:3:LYS:NZ	1.77	0.98
1:F:19:VAL:HG13	4:F:394:HOH:O	1.66	0.95
1:F:139:ARG:HD3	4:F:389:HOH:O	1.66	0.95
1:B:3:LYS:HZ2	1:B:3:LYS:HA	1.33	0.93
1:B:3:LYS:HA	1:B:3:LYS:NZ	1.85	0.92
1:D:74:SER:H	1:D:82:ASN:HD22	1.21	0.87
1:D:3:LYS:NZ	1:D:3:LYS:HA	1.89	0.87
1:A:3:LYS:HA	1:A:3:LYS:NZ	1.89	0.87
1:E:34:GLU:HA	1:E:87:THR:HB	1.57	0.86
1:C:27:MET:HG3	4:C:996:HOH:O	1.75	0.86
1:D:136:ARG:HD3	4:D:384:HOH:O	1.76	0.85
1:A:136:ARG:HD3	4:A:1003:HOH:O	1.78	0.83
1:C:3:LYS:HZ2	1:C:3:LYS:HA	1.43	0.83
1:D:34:GLU:HA	1:D:87:THR:HB	1.59	0.82
1:D:3:LYS:HA	1:D:3:LYS:HZ2	1.41	0.82
1:C:3:LYS:HA	1:C:3:LYS:NZ	1.95	0.81
1:F:11:THR:OG1	1:F:14:GLU:HG3	1.81	0.81
1:C:34:GLU:HA	1:C:87:THR:HB	1.63	0.80
1:C:108:ARG:HH11	1:C:108:ARG:HB3	1.44	0.80
1:A:11:THR:OG1	1:A:14:GLU:HG3	1.82	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:PHE:O	4:E:992:HOH:O	1.99	0.79
1:F:34:GLU:HA	1:F:87:THR:HB	1.64	0.79
1:A:34:GLU:HA	1:A:87:THR:HB	1.65	0.79
1:F:108:ARG:HH11	1:F:108:ARG:HB3	1.48	0.78
1:F:111:VAL:HA	4:F:394:HOH:O	1.86	0.76
1:D:108:ARG:HH11	1:D:108:ARG:HB3	1.51	0.75
1:F:3:LYS:NZ	1:F:3:LYS:HA	2.03	0.74
1:B:22:GLY:HA2	3:B:901:GOL:O1	1.88	0.73
1:B:34:GLU:HA	1:B:87:THR:HB	1.70	0.73
1:B:216:VAL:HA	4:B:969:HOH:O	1.88	0.72
1:D:214:PHE:HA	1:D:215:PRO:C	2.14	0.72
1:B:108:ARG:HB3	1:B:108:ARG:HH11	1.55	0.72
1:D:74:SER:H	1:D:82:ASN:ND2	1.88	0.72
1:D:188:LEU:HD11	1:D:197:LEU:HD21	1.73	0.71
1:D:38:HIS:O	4:D:316:HOH:O	2.08	0.70
1:C:188:LEU:HD11	1:C:197:LEU:HD21	1.74	0.70
1:C:12:TRP:HD1	4:D:387:HOH:O	1.73	0.69
1:B:259:PRO:O	4:B:954:HOH:O	2.09	0.69
1:D:74:SER:N	1:D:82:ASN:HD22	1.89	0.69
1:D:47:LEU:HD12	1:D:187:MET:HE1	1.75	0.69
1:A:74:SER:H	1:A:82:ASN:HD22	1.39	0.69
1:F:74:SER:H	1:F:82:ASN:HD22	1.39	0.69
1:A:108:ARG:HH11	1:A:108:ARG:HB3	1.57	0.68
1:B:183:GLU:O	1:B:187:MET:HB2	1.93	0.68
1:C:74:SER:H	1:C:82:ASN:HD22	1.43	0.66
1:E:74:SER:H	1:E:82:ASN:HD22	1.44	0.66
1:B:159:ASP:OD2	1:B:161:ALA:HB3	1.96	0.66
1:E:5:VAL:HG22	4:E:928:HOH:O	1.96	0.66
1:C:203:HIS:HE1	1:C:226:THR:OG1	1.79	0.65
1:D:36:HIS:N	4:D:387:HOH:O	2.30	0.65
1:A:188:LEU:C	4:A:1012:HOH:O	2.39	0.65
1:B:74:SER:H	1:B:82:ASN:HD22	1.43	0.64
1:E:23:ASP:HB2	1:E:113:ARG:NH1	2.12	0.64
1:C:191:TYR:HA	4:C:1021:HOH:O	1.97	0.64
1:D:172:LEU:HB3	1:D:176:ILE:HD11	1.79	0.64
1:A:190:LEU:N	4:A:1012:HOH:O	2.30	0.64
1:E:11:THR:OG1	1:E:14:GLU:HG3	1.98	0.64
1:A:136:ARG:CD	4:A:1003:HOH:O	2.42	0.63
1:B:11:THR:OG1	1:B:14:GLU:HG3	1.97	0.63
1:D:23:ASP:HB2	1:D:113:ARG:NH1	2.13	0.63
1:F:108:ARG:HB3	1:F:108:ARG:NH1	2.13	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:PHE:HA	1:C:215:PRO:C	2.23	0.63
1:F:188:LEU:HD11	1:F:197:LEU:HD21	1.79	0.63
1:B:188:LEU:HD21	1:B:197:LEU:HD23	1.80	0.63
1:C:240:LEU:O	1:C:244:VAL:HG23	1.99	0.63
1:F:23:ASP:HB2	1:F:113:ARG:NH1	2.14	0.63
1:C:23:ASP:HB2	1:C:113:ARG:NH1	2.13	0.63
1:E:256:GLU:C	1:E:258:PRO:HD3	2.25	0.62
1:A:255:GLN:NE2	4:A:995:HOH:O	2.31	0.62
1:A:137:GLU:HG2	1:C:140:TYR:OH	2.00	0.62
1:F:216:VAL:HG12	4:F:343:HOH:O	1.99	0.62
1:C:104:ARG:HD3	1:C:137:GLU:OE2	1.99	0.61
1:C:172:LEU:HB3	1:C:176:ILE:HD11	1.81	0.61
1:D:203:HIS:HE1	1:D:226:THR:OG1	1.83	0.61
1:C:199:ARG:NH1	4:C:1012:HOH:O	2.33	0.61
1:A:104:ARG:HD3	1:A:137:GLU:OE2	2.00	0.61
1:D:28:LEU:HD23	1:D:116:LEU:HD21	1.82	0.61
1:E:69:GLN:H	3:E:903:GOL:H11	1.66	0.61
1:C:75:GLN:HG2	1:C:122:GLU:HG2	1.83	0.60
1:C:159:ASP:OD2	1:C:161:ALA:HB3	2.02	0.60
1:D:13:LYS:NZ	4:D:413:HOH:O	2.34	0.60
1:B:187:MET:HE3	1:B:191:TYR:HB2	1.84	0.60
1:D:37:GLY:N	4:D:387:HOH:O	2.34	0.60
1:C:11:THR:OG1	1:C:14:GLU:HG3	2.01	0.60
1:C:166:LEU:HD22	1:C:240:LEU:HD23	1.84	0.60
1:B:213:VAL:O	4:B:969:HOH:O	2.16	0.60
1:A:172:LEU:HB3	1:A:176:ILE:HD11	1.84	0.59
1:F:111:VAL:CA	4:F:394:HOH:O	2.44	0.59
1:A:37:GLY:HA2	1:A:224:PRO:O	2.02	0.59
1:B:256:GLU:C	1:B:258:PRO:HD3	2.27	0.59
1:A:188:LEU:HD21	1:A:197:LEU:HD23	1.84	0.59
1:D:240:LEU:O	1:D:244:VAL:HG23	2.03	0.59
1:C:120:HIS:HB3	1:C:123:ASN:ND2	2.17	0.59
1:B:120:HIS:HB3	1:B:123:ASN:ND2	2.18	0.59
1:C:256:GLU:C	1:C:258:PRO:HD3	2.27	0.59
1:F:136:ARG:HD3	4:F:428:HOH:O	2.02	0.59
1:C:118:ASN:ND2	1:C:120:HIS:H	2.00	0.58
1:F:256:GLU:C	1:F:258:PRO:HD3	2.28	0.58
1:A:83:HIS:HE1	4:A:957:HOH:O	1.85	0.58
1:F:172:LEU:HB3	1:F:176:ILE:HD11	1.85	0.58
1:B:223:ALA:N	4:B:972:HOH:O	2.30	0.58
1:E:108:ARG:HH11	1:E:108:ARG:HB3	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ARG:HB3	1:B:108:ARG:NH1	2.19	0.58
1:F:38:HIS:HB3	4:F:405:HOH:O	2.04	0.58
1:A:108:ARG:HB3	1:A:108:ARG:NH1	2.19	0.58
1:A:187:MET:O	4:A:1012:HOH:O	2.17	0.58
1:A:159:ASP:OD2	1:A:161:ALA:HB3	2.04	0.58
1:D:256:GLU:C	1:D:258:PRO:HD3	2.29	0.57
1:D:6:PHE:HE1	1:D:54:GLN:NE2	2.02	0.57
1:E:188:LEU:HD11	1:E:197:LEU:HD21	1.85	0.56
1:F:3:LYS:HA	1:F:3:LYS:HZ2	1.68	0.56
1:A:256:GLU:C	1:A:258:PRO:HD3	2.31	0.56
1:C:62:ALA:HB1	4:C:996:HOH:O	2.04	0.56
1:D:224:PRO:HA	4:D:382:HOH:O	2.04	0.56
1:E:214:PHE:HA	1:E:215:PRO:C	2.30	0.56
1:C:56:VAL:O	1:C:60:ILE:HG12	2.05	0.56
1:C:118:ASN:ND2	1:C:123:ASN:HD22	2.03	0.56
1:E:172:LEU:HB3	1:E:176:ILE:HD11	1.87	0.56
1:F:83:HIS:HE1	4:F:398:HOH:O	1.88	0.55
1:B:188:LEU:HD21	1:B:197:LEU:CD2	2.36	0.55
1:D:159:ASP:OD2	1:D:161:ALA:HB3	2.07	0.55
1:C:108:ARG:HB3	1:C:108:ARG:NH1	2.17	0.55
1:D:188:LEU:O	1:D:192:PRO:HG3	2.07	0.55
1:C:11:THR:HB	4:D:383:HOH:O	2.06	0.55
1:D:5:VAL:HG22	4:D:350:HOH:O	2.07	0.55
1:F:235:ARG:HD2	4:F:367:HOH:O	2.06	0.55
1:F:166:LEU:HD22	1:F:240:LEU:HD23	1.89	0.55
1:C:166:LEU:C	1:C:168:PRO:HD3	2.32	0.55
1:F:214:PHE:HA	1:F:215:PRO:C	2.32	0.55
1:D:47:LEU:CD1	1:D:187:MET:HE1	2.37	0.54
1:A:35:GLN:NE2	1:A:37:GLY:H	2.06	0.54
1:F:75:GLN:HG2	1:F:122:GLU:HG2	1.88	0.54
1:E:18:ARG:NE	4:E:961:HOH:O	2.25	0.54
1:E:260:THR:HA	4:E:1026:HOH:O	2.07	0.54
1:D:172:LEU:CB	1:D:176:ILE:HD11	2.38	0.54
1:E:159:ASP:OD2	1:E:161:ALA:HB3	2.08	0.54
1:A:8:GLY:O	1:B:41:CYS:HB2	2.07	0.54
1:A:188:LEU:HD11	1:A:197:LEU:HD21	1.89	0.54
1:F:172:LEU:CB	1:F:176:ILE:HD11	2.38	0.54
1:B:23:ASP:HB2	1:B:113:ARG:NH1	2.23	0.54
1:B:83:HIS:CD2	1:B:83:HIS:H	2.26	0.54
1:B:113:ARG:NH1	4:B:923:HOH:O	2.41	0.54
1:E:162:VAL:HG12	1:E:166:LEU:HD23	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:VAL:N	4:F:394:HOH:O	2.40	0.54
1:A:120:HIS:HB3	1:A:123:ASN:ND2	2.23	0.53
1:B:72:TYR:CG	1:B:73:LYS:N	2.77	0.53
1:B:166:LEU:CD2	1:B:240:LEU:HD23	2.38	0.53
1:F:3:LYS:HA	1:F:3:LYS:HZ3	1.74	0.53
1:F:159:ASP:OD2	1:F:161:ALA:HB3	2.08	0.53
1:A:191:TYR:N	4:A:1012:HOH:O	2.41	0.53
1:B:167:TYR:O	1:B:169:GLU:N	2.42	0.53
1:A:188:LEU:HD21	1:A:197:LEU:CD2	2.39	0.53
1:D:188:LEU:HD21	1:D:197:LEU:CD2	2.39	0.53
1:B:75:GLN:HG2	1:B:122:GLU:HG2	1.90	0.53
1:D:162:VAL:HG12	1:D:166:LEU:HD23	1.90	0.53
1:B:166:LEU:C	1:B:168:PRO:HD3	2.33	0.53
1:B:166:LEU:HD22	1:B:240:LEU:HD23	1.90	0.53
1:D:168:PRO:O	1:D:169:GLU:HB2	2.09	0.53
1:E:167:TYR:O	1:E:169:GLU:N	2.42	0.53
1:B:172:LEU:HB3	1:B:176:ILE:HD11	1.91	0.53
1:C:188:LEU:HD21	1:C:197:LEU:HD23	1.91	0.53
1:E:203:HIS:HE1	1:E:226:THR:OG1	1.90	0.53
1:A:214:PHE:HA	1:A:215:PRO:C	2.33	0.53
1:B:197:LEU:HD13	1:B:200:VAL:HG21	1.90	0.53
1:F:166:LEU:C	1:F:168:PRO:HD3	2.33	0.53
1:A:223:ALA:N	1:A:224:PRO:CD	2.72	0.52
1:A:172:LEU:HB2	4:A:1006:HOH:O	2.10	0.52
1:C:166:LEU:CD2	1:C:240:LEU:HD23	2.40	0.52
1:A:166:LEU:C	1:A:168:PRO:HD3	2.35	0.52
1:E:120:HIS:HA	4:E:905:HOH:O	2.09	0.52
1:B:214:PHE:HA	1:B:215:PRO:C	2.34	0.52
1:E:3:LYS:HA	1:E:3:LYS:HZ3	1.69	0.52
1:C:162:VAL:HG12	1:C:166:LEU:HD23	1.91	0.52
1:F:108:ARG:HH11	1:F:108:ARG:CB	2.19	0.52
1:D:108:ARG:HB3	1:D:108:ARG:NH1	2.23	0.52
1:F:120:HIS:HB3	1:F:123:ASN:ND2	2.25	0.52
1:B:260:THR:HA	4:B:954:HOH:O	2.10	0.52
1:B:104:ARG:HD3	1:B:137:GLU:OE2	2.10	0.51
1:B:120:HIS:HA	4:B:904:HOH:O	2.10	0.51
1:A:172:LEU:CB	1:A:176:ILE:HD11	2.40	0.51
1:C:37:GLY:HA2	1:C:224:PRO:O	2.10	0.51
1:C:35:GLN:NE2	1:C:37:GLY:H	2.08	0.51
1:C:77:LYS:NZ	4:C:920:HOH:O	2.43	0.51
1:D:52:VAL:O	1:D:56:VAL:HG23	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:LEU:C	1:E:168:PRO:HD3	2.35	0.51
1:E:188:LEU:O	1:E:192:PRO:HG3	2.10	0.51
1:E:120:HIS:HB3	1:E:123:ASN:ND2	2.25	0.51
1:C:188:LEU:O	1:C:192:PRO:HG3	2.10	0.51
1:D:188:LEU:HD21	1:D:197:LEU:HD23	1.92	0.51
1:E:83:HIS:H	1:E:83:HIS:CD2	2.27	0.51
1:F:166:LEU:CD2	1:F:240:LEU:HD23	2.40	0.51
1:A:75:GLN:HG2	1:A:122:GLU:HG2	1.92	0.51
1:F:240:LEU:O	1:F:244:VAL:HG23	2.11	0.51
1:B:3:LYS:HA	1:B:3:LYS:HZ3	1.76	0.50
1:E:35:GLN:HB2	1:F:12:TRP:CD1	2.45	0.50
1:E:83:HIS:HE1	4:E:941:HOH:O	1.94	0.50
1:A:168:PRO:O	1:A:169:GLU:HB2	2.11	0.50
1:A:183:GLU:O	1:A:187:MET:HB2	2.11	0.50
1:B:217:ASP:N	4:B:969:HOH:O	2.44	0.50
1:A:57:ALA:HB1	1:A:62:ALA:O	2.12	0.50
1:B:137:GLU:HG2	1:F:140:TYR:OH	2.12	0.50
1:F:203:HIS:HE1	1:F:226:THR:OG1	1.95	0.50
1:E:47:LEU:HD12	1:E:187:MET:HE1	1.94	0.50
1:A:87:THR:HG21	4:A:906:HOH:O	2.12	0.50
1:E:47:LEU:CD1	1:E:187:MET:HE1	2.42	0.50
1:C:10:LEU:O	1:D:41:CYS:HA	2.12	0.50
1:C:76:GLN:HG3	1:C:221:THR:OG1	2.12	0.50
1:D:230:ALA:N	4:D:379:HOH:O	2.33	0.50
1:A:41:CYS:HB2	1:B:8:GLY:O	2.12	0.49
1:E:3:LYS:NZ	1:E:3:LYS:CA	2.64	0.49
1:A:83:HIS:H	1:A:83:HIS:CD2	2.30	0.49
1:E:188:LEU:HD21	1:E:197:LEU:HD23	1.94	0.49
1:F:104:ARG:HD3	1:F:137:GLU:OE2	2.12	0.49
1:B:188:LEU:HD11	1:B:197:LEU:HD21	1.93	0.49
1:B:188:LEU:O	1:B:192:PRO:HG3	2.12	0.49
1:D:214:PHE:CA	1:D:215:PRO:C	2.85	0.49
1:D:3:LYS:HA	1:D:3:LYS:HZ3	1.75	0.49
1:B:37:GLY:HA2	1:B:224:PRO:O	2.13	0.49
1:B:140:TYR:O	4:B:908:HOH:O	2.19	0.49
1:C:165:ARG:NE	4:C:988:HOH:O	2.45	0.49
1:A:197:LEU:HD13	1:A:200:VAL:HG21	1.93	0.49
1:B:203:HIS:HE1	1:B:226:THR:OG1	1.96	0.49
1:E:104:ARG:HD3	1:E:137:GLU:OE2	2.13	0.49
1:F:188:LEU:HD21	1:F:197:LEU:HD23	1.94	0.48
1:F:101:ASP:OD1	1:F:104:ARG:NH2	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:PRO:HD2	4:C:1021:HOH:O	2.13	0.48
1:C:12:TRP:CD1	1:D:35:GLN:HB2	2.48	0.48
1:D:166:LEU:C	1:D:168:PRO:HD3	2.39	0.48
1:D:218:PRO:O	4:D:378:HOH:O	2.20	0.48
1:B:108:ARG:HH11	1:B:108:ARG:CB	2.24	0.48
1:E:35:GLN:NE2	1:E:37:GLY:H	2.12	0.48
1:E:183:GLU:O	1:E:187:MET:HB2	2.13	0.48
1:C:35:GLN:HB2	1:D:12:TRP:CD1	2.49	0.48
1:C:172:LEU:CB	1:C:176:ILE:HD11	2.43	0.48
1:F:183:GLU:O	1:F:187:MET:HB2	2.13	0.48
1:B:140:TYR:OH	1:D:137:GLU:HG2	2.13	0.48
1:C:28:LEU:HD23	1:C:116:LEU:HD21	1.96	0.48
1:D:28:LEU:HD23	1:D:116:LEU:CD2	2.44	0.48
1:E:168:PRO:O	1:E:169:GLU:HB2	2.14	0.48
1:F:30:VAL:HG11	1:F:127:ILE:HD11	1.96	0.48
1:C:108:ARG:HA	4:C:1013:HOH:O	2.14	0.47
1:D:210:PRO:HG3	1:E:158:LYS:HD3	1.96	0.47
1:C:72:TYR:CG	1:C:73:LYS:N	2.82	0.47
1:E:136:ARG:CD	4:E:962:HOH:O	2.34	0.47
1:F:162:VAL:HG12	1:F:166:LEU:HD23	1.97	0.47
1:C:183:GLU:O	1:C:187:MET:HB2	2.14	0.47
1:D:166:LEU:HD22	1:D:240:LEU:HD23	1.96	0.47
1:E:197:LEU:HD13	1:E:200:VAL:HG21	1.97	0.47
1:D:3:LYS:HE3	4:D:357:HOH:O	2.13	0.47
1:C:66:PRO:HA	4:C:992:HOH:O	2.14	0.47
1:D:35:GLN:NE2	1:D:37:GLY:H	2.13	0.47
1:A:101:ASP:OD1	1:A:104:ARG:NH2	2.47	0.47
1:D:104:ARG:HB3	4:D:393:HOH:O	2.15	0.47
1:D:183:GLU:O	1:D:187:MET:HB2	2.16	0.46
1:F:116:LEU:CD1	1:F:131:ILE:HD11	2.45	0.46
1:B:172:LEU:CB	1:B:176:ILE:HD11	2.45	0.46
1:C:197:LEU:HD13	1:C:200:VAL:HG21	1.97	0.46
1:D:166:LEU:CD2	1:D:240:LEU:HD23	2.45	0.46
1:A:23:ASP:HB2	1:A:113:ARG:NH1	2.30	0.46
1:C:167:TYR:O	1:C:169:GLU:N	2.48	0.46
1:D:23:ASP:HA	4:D:394:HOH:O	2.15	0.46
1:D:120:HIS:HB3	1:D:123:ASN:ND2	2.31	0.46
1:C:108:ARG:HH11	1:C:108:ARG:CB	2.22	0.46
1:A:166:LEU:HD22	1:A:240:LEU:HD23	1.98	0.46
1:C:82:ASN:ND2	1:C:89:SER:OG	2.46	0.46
1:A:47:LEU:CD1	1:A:187:MET:HE1	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:CYS:SG	1:B:194:LEU:HB3	2.56	0.45
1:A:68:LEU:HA	3:A:902:GOL:H11	1.99	0.45
1:D:188:LEU:HD23	1:D:195:VAL:CG1	2.46	0.45
1:F:87:THR:HG21	4:F:361:HOH:O	2.16	0.45
1:A:203:HIS:HE1	1:A:226:THR:OG1	2.00	0.45
1:B:117:MET:HE2	1:B:249:ILE:HD13	1.98	0.45
1:C:196:ASP:OD2	1:C:199:ARG:HG3	2.16	0.45
1:D:72:TYR:CG	1:D:73:LYS:N	2.84	0.45
1:F:168:PRO:O	1:F:169:GLU:HB2	2.15	0.45
1:C:118:ASN:HD21	1:C:123:ASN:HD22	1.65	0.45
1:A:203:HIS:HD2	1:A:204:PRO:O	2.00	0.45
1:C:223:ALA:HB3	1:C:224:PRO:HD3	1.99	0.45
1:E:108:ARG:HB3	1:E:108:ARG:NH1	2.30	0.45
1:A:45:ASP:O	1:A:49:PRO:HG3	2.17	0.45
1:B:28:LEU:HD23	1:B:116:LEU:HD21	1.98	0.45
1:C:41:CYS:SG	1:C:194:LEU:HB3	2.57	0.45
1:C:47:LEU:CD1	1:C:187:MET:HE1	2.47	0.45
1:E:172:LEU:CB	1:E:176:ILE:HD11	2.46	0.45
1:A:167:TYR:O	1:A:169:GLU:N	2.50	0.44
1:B:137:GLU:O	1:B:140:TYR:HB2	2.17	0.44
1:D:83:HIS:CD2	1:D:83:HIS:H	2.35	0.44
1:C:188:LEU:HD21	1:C:197:LEU:CD2	2.47	0.44
1:A:28:LEU:HD23	1:A:116:LEU:HD21	1.99	0.44
1:C:257:PHE:N	1:C:258:PRO:HD3	2.33	0.44
1:E:235:ARG:O	1:E:239:GLU:HG2	2.18	0.44
1:B:196:ASP:OD2	1:B:199:ARG:HG3	2.18	0.44
1:D:140:TYR:CE1	1:F:137:GLU:HG2	2.53	0.44
1:C:203:HIS:CE1	1:C:226:THR:OG1	2.65	0.44
1:D:162:VAL:HG11	1:D:244:VAL:HG21	2.00	0.43
1:F:35:GLN:NE2	1:F:37:GLY:H	2.16	0.43
1:C:106:LEU:O	1:C:109:HIS:HB2	2.18	0.43
1:D:11:THR:OG1	1:D:14:GLU:HG3	2.19	0.43
1:D:75:GLN:HG2	1:D:122:GLU:HG2	2.00	0.43
1:E:75:GLN:HG2	1:E:122:GLU:HG2	2.01	0.43
1:A:223:ALA:HB3	1:A:224:PRO:HD3	2.01	0.43
1:B:137:GLU:HG2	1:F:140:TYR:CZ	2.53	0.43
1:C:83:HIS:H	1:C:83:HIS:CD2	2.36	0.43
1:B:203:HIS:HD2	1:B:204:PRO:O	2.02	0.43
1:F:82:ASN:ND2	1:F:89:SER:OG	2.45	0.43
1:E:28:LEU:HD23	1:E:116:LEU:HD21	2.00	0.43
1:A:35:GLN:HB2	1:B:12:TRP:CD1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:HIS:HA	4:C:907:HOH:O	2.18	0.43
1:C:162:VAL:HG11	1:C:244:VAL:HG21	2.01	0.43
1:A:50:THR:HB	4:A:935:HOH:O	2.19	0.43
1:A:210:PRO:HG3	1:F:158:LYS:CD	2.49	0.43
1:E:166:LEU:HD22	1:E:240:LEU:HD23	2.01	0.43
1:A:74:SER:H	1:A:82:ASN:ND2	2.13	0.42
1:A:162:VAL:HG12	1:A:166:LEU:HD23	2.00	0.42
1:A:260:THR:HG22	1:A:260:THR:O	2.19	0.42
1:B:232:THR:HG23	4:B:997:HOH:O	2.19	0.42
1:E:76:GLN:NE2	1:E:220:ARG:HB2	2.34	0.42
1:F:118:ASN:ND2	1:F:123:ASN:HD22	2.17	0.42
1:C:101:ASP:OD1	1:C:104:ARG:NH2	2.50	0.42
1:F:83:HIS:CD2	1:F:83:HIS:H	2.37	0.42
1:A:187:MET:HE3	1:A:191:TYR:HB2	2.01	0.42
1:A:249:ILE:O	1:A:253:ILE:HG13	2.19	0.42
1:B:74:SER:H	1:B:82:ASN:ND2	2.14	0.42
1:C:207:THR:HG22	4:C:985:HOH:O	2.18	0.42
1:D:108:ARG:HH11	1:D:108:ARG:CB	2.28	0.42
1:F:116:LEU:HD13	1:F:131:ILE:HD11	2.02	0.42
1:F:257:PHE:N	1:F:258:PRO:HD3	2.35	0.42
1:C:47:LEU:HD12	1:C:187:MET:HE1	2.02	0.42
1:D:158:LYS:HD3	1:E:210:PRO:HG3	2.01	0.42
1:D:167:TYR:O	1:D:169:GLU:N	2.53	0.42
1:E:87:THR:HG21	4:E:914:HOH:O	2.18	0.42
1:F:48:LEU:HD23	1:F:48:LEU:HA	1.82	0.42
1:F:72:TYR:CG	1:F:73:LYS:N	2.87	0.42
1:F:196:ASP:OD2	1:F:199:ARG:HG3	2.19	0.42
1:B:46:VAL:HG21	1:B:69:GLN:HA	2.02	0.42
1:C:117:MET:HE2	1:C:249:ILE:HD13	2.02	0.42
1:A:72:TYR:CG	1:A:73:LYS:N	2.88	0.42
1:A:210:PRO:HG3	1:F:158:LYS:HD3	2.02	0.42
1:B:118:ASN:HD21	1:B:123:ASN:HD22	1.68	0.42
1:D:191:TYR:HB3	1:D:194:LEU:HD12	2.02	0.41
1:F:118:ASN:HD21	1:F:123:ASN:HD22	1.67	0.41
1:F:37:GLY:HA2	1:F:224:PRO:O	2.20	0.41
1:F:167:TYR:O	1:F:169:GLU:N	2.53	0.41
1:A:196:ASP:HA	4:A:939:HOH:O	2.19	0.41
1:B:23:ASP:N	3:B:901:GOL:H2	2.35	0.41
1:D:197:LEU:HA	1:D:200:VAL:HG23	2.01	0.41
1:F:197:LEU:HD13	1:F:200:VAL:HG21	2.02	0.41
1:B:162:VAL:HG12	1:B:166:LEU:HD23	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:O	1:B:244:VAL:HG23	2.20	0.41
1:C:168:PRO:O	1:C:169:GLU:HB2	2.19	0.41
1:D:252:ALA:HB1	1:E:211:TYR:CE2	2.56	0.41
1:E:188:LEU:HD21	1:E:197:LEU:CD2	2.50	0.41
1:E:203:HIS:HD2	1:E:204:PRO:O	2.04	0.41
1:A:138:LEU:HD12	1:A:138:LEU:HA	1.84	0.41
1:B:168:PRO:O	1:B:169:GLU:HB2	2.20	0.41
1:C:137:GLU:O	1:C:140:TYR:HB2	2.21	0.41
1:A:209:PRO:HD2	4:A:980:HOH:O	2.20	0.41
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.81	0.41
1:C:68:LEU:HA	3:C:904:GOL:H11	2.02	0.41
1:D:56:VAL:O	1:D:60:ILE:HG12	2.21	0.41
1:D:258:PRO:HA	1:D:259:PRO:HD3	1.98	0.41
1:A:188:LEU:O	1:A:192:PRO:HG3	2.21	0.41
1:C:151:LEU:C	1:C:151:LEU:HD12	2.46	0.41
1:D:131:ILE:CD1	1:D:150:VAL:CG2	2.99	0.41
1:D:203:HIS:HD2	1:D:204:PRO:O	2.04	0.41
1:E:39:HIS:CD2	1:E:40:MET:HG3	2.56	0.41
1:A:108:ARG:HH11	1:A:108:ARG:CB	2.27	0.41
1:B:35:GLN:NE2	1:B:37:GLY:H	2.18	0.41
1:D:158:LYS:CD	1:E:210:PRO:HG3	2.51	0.41
1:A:196:ASP:OD2	1:A:199:ARG:HG3	2.22	0.40
1:B:223:ALA:N	1:B:224:PRO:CD	2.84	0.40
1:E:72:TYR:CG	1:E:73:LYS:N	2.89	0.40
1:A:235:ARG:O	1:A:239:GLU:HG2	2.21	0.40
1:D:203:HIS:CE1	1:D:226:THR:OG1	2.69	0.40
1:B:176:ILE:HD12	1:B:205:PRO:HB3	2.04	0.40
1:E:235:ARG:HG2	1:E:235:ARG:NH1	2.37	0.40
1:A:166:LEU:CD2	1:A:240:LEU:HD23	2.51	0.40
1:D:3:LYS:HG2	4:D:401:HOH:O	2.21	0.40
1:F:41:CYS:SG	1:F:194:LEU:HB3	2.61	0.40

All (1) 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)
4:D:314:HOH:O	4:F:405:HOH:O[1_655]	1.85	0.35

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	257/259 (99%)	243 (95%)	13 (5%)	1 (0%)	30	28
1	B	257/259 (99%)	242 (94%)	13 (5%)	2 (1%)	16	12
1	C	257/259 (99%)	241 (94%)	14 (5%)	2 (1%)	16	12
1	D	257/259 (99%)	243 (95%)	12 (5%)	2 (1%)	16	12
1	E	257/259 (99%)	244 (95%)	12 (5%)	1 (0%)	30	28
1	F	257/259 (99%)	243 (95%)	13 (5%)	1 (0%)	30	28
All	All	1542/1554 (99%)	1456 (94%)	77 (5%)	9 (1%)	21	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	GLU
1	B	169	GLU
1	C	169	GLU
1	D	169	GLU
1	E	169	GLU
1	F	169	GLU
1	D	3	LYS
1	C	3	LYS
1	B	168	PRO

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	214/214 (100%)	207 (97%)	7 (3%)	33	37
1	B	214/214 (100%)	206 (96%)	8 (4%)	30	33
1	C	214/214 (100%)	207 (97%)	7 (3%)	33	37
1	D	214/214 (100%)	204 (95%)	10 (5%)	23	24
1	E	214/214 (100%)	207 (97%)	7 (3%)	33	37
1	F	214/214 (100%)	207 (97%)	7 (3%)	33	37
All	All	1284/1284 (100%)	1238 (96%)	46 (4%)	31	34

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	35	GLN
1	A	87	THR
1	A	138	LEU
1	A	165	ARG
1	A	166	LEU
1	A	243	GLU
1	B	3	LYS
1	B	35	GLN
1	B	87	THR
1	B	138	LEU
1	B	165	ARG
1	B	166	LEU
1	B	212	ASP
1	B	243	GLU
1	C	3	LYS
1	C	35	GLN
1	C	87	THR
1	C	108	ARG
1	C	138	LEU
1	C	165	ARG
1	C	166	LEU
1	D	3	LYS
1	D	35	GLN
1	D	82	ASN
1	D	87	THR
1	D	108	ARG
1	D	138	LEU
1	D	165	ARG
1	D	166	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	195	VAL
1	D	207	THR
1	E	3	LYS
1	E	35	GLN
1	E	82	ASN
1	E	87	THR
1	E	138	LEU
1	E	165	ARG
1	E	166	LEU
1	F	3	LYS
1	F	35	GLN
1	F	87	THR
1	F	108	ARG
1	F	138	LEU
1	F	165	ARG
1	F	166	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	82	ASN
1	A	83	HIS
1	A	118	ASN
1	A	203	HIS
1	A	255	GLN
1	B	35	GLN
1	B	76	GLN
1	B	82	ASN
1	B	83	HIS
1	B	118	ASN
1	B	203	HIS
1	B	255	GLN
1	C	35	GLN
1	C	54	GLN
1	C	82	ASN
1	C	83	HIS
1	C	118	ASN
1	C	203	HIS
1	C	255	GLN
1	D	35	GLN
1	D	54	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	76	GLN
1	D	82	ASN
1	D	83	HIS
1	D	118	ASN
1	D	203	HIS
1	D	255	GLN
1	E	35	GLN
1	E	76	GLN
1	E	82	ASN
1	E	83	HIS
1	E	118	ASN
1	E	203	HIS
1	E	255	GLN
1	F	35	GLN
1	F	54	GLN
1	F	76	GLN
1	F	82	ASN
1	F	83	HIS
1	F	118	ASN
1	F	203	HIS
1	F	255	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](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	GOL	E	903	-	5,5,5	0.44	0	5,5,5	0.49	0
3	GOL	C	904	-	5,5,5	0.45	0	5,5,5	0.55	0
3	GOL	B	901	-	5,5,5	0.33	0	5,5,5	0.56	0
3	GOL	A	902	-	5,5,5	0.73	0	5,5,5	0.97	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
3	GOL	E	903	-	-	0/4/4/4	-
3	GOL	C	904	-	-	0/4/4/4	-
3	GOL	B	901	-	-	0/4/4/4	-
3	GOL	A	902	-	-	0/4/4/4	-

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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	903	GOL	1	0
3	C	904	GOL	1	0
3	B	901	GOL	2	0
3	A	902	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	259/259 (100%)	0.53	16 (6%)	26	28	22, 40, 68, 85	0
1	B	259/259 (100%)	0.54	12 (4%)	37	39	23, 40, 68, 85	0
1	C	259/259 (100%)	0.62	24 (9%)	14	15	22, 40, 68, 86	0
1	D	259/259 (100%)	0.67	21 (8%)	18	19	21, 39, 68, 86	0
1	E	259/259 (100%)	0.34	15 (5%)	29	30	21, 38, 68, 85	0
1	F	259/259 (100%)	0.28	17 (6%)	24	26	20, 38, 67, 85	0
All	All	1554/1554 (100%)	0.50	105 (6%)	23	25	20, 39, 68, 86	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	3	LYS	4.5
1	E	172	LEU	4.4
1	F	172	LEU	4.2
1	F	197	LEU	3.8
1	C	260	THR	3.7
1	D	172	LEU	3.7
1	D	194	LEU	3.7
1	D	195	VAL	3.7
1	A	172	LEU	3.7
1	C	2	SER	3.7
1	D	200	VAL	3.6
1	C	172	LEU	3.6
1	A	2	SER	3.5
1	A	21	ALA	3.5
1	B	172	LEU	3.5
1	E	2	SER	3.5
1	B	260	THR	3.5
1	D	188	LEU	3.4
1	E	166	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	260	THR	3.3
1	D	201	VAL	3.3
1	F	163	ILE	3.3
1	B	166	LEU	3.3
1	F	168	PRO	3.2
1	D	230	ALA	3.2
1	F	21	ALA	3.2
1	A	166	LEU	3.1
1	C	167	TYR	3.1
1	E	171	PHE	3.1
1	A	259	PRO	3.1
1	C	22	GLY	3.1
1	A	260	THR	3.1
1	C	188	LEU	3.0
1	D	197	LEU	2.9
1	E	260	THR	2.8
1	C	259	PRO	2.8
1	F	2	SER	2.8
1	E	197	LEU	2.8
1	F	166	LEU	2.8
1	F	260	THR	2.8
1	F	259	PRO	2.8
1	C	168	PRO	2.7
1	D	166	LEU	2.7
1	B	201	VAL	2.7
1	D	2	SER	2.7
1	E	168	PRO	2.7
1	B	167	TYR	2.7
1	D	167	TYR	2.7
1	B	200	VAL	2.7
1	C	240	LEU	2.6
1	A	171	PHE	2.6
1	D	168	PRO	2.6
1	D	224	PRO	2.6
1	D	176	ILE	2.6
1	E	259	PRO	2.5
1	C	163	ILE	2.5
1	E	164	GLN	2.5
1	C	166	LEU	2.5
1	B	3	LYS	2.5
1	B	259	PRO	2.4
1	A	162	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	20	ALA	2.4
1	C	171	PHE	2.4
1	D	162	VAL	2.4
1	F	162	VAL	2.4
1	E	201	VAL	2.3
1	A	167	TYR	2.3
1	D	173	GLY	2.3
1	E	23	ASP	2.3
1	F	194	LEU	2.3
1	F	235	ARG	2.3
1	D	181	VAL	2.3
1	E	195	VAL	2.3
1	A	161	ALA	2.3
1	C	197	LEU	2.3
1	F	171	PHE	2.2
1	E	200	VAL	2.2
1	C	175	ASP	2.2
1	F	23	ASP	2.2
1	C	57	ALA	2.2
1	F	22	GLY	2.2
1	F	174	TRP	2.2
1	B	229	SER	2.2
1	B	171	PHE	2.2
1	D	171	PHE	2.2
1	A	160	PRO	2.2
1	D	233	ALA	2.2
1	C	60	ILE	2.2
1	D	241	ILE	2.2
1	A	175	ASP	2.1
1	C	21	ALA	2.1
1	A	188	LEU	2.1
1	C	3	LYS	2.1
1	C	170	GLY	2.1
1	C	200	VAL	2.1
1	B	194	LEU	2.1
1	C	235	ARG	2.1
1	A	163	ILE	2.1
1	A	12	TRP	2.1
1	F	121	TYR	2.0
1	B	181	VAL	2.0
1	C	201	VAL	2.0
1	C	244	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	189	ALA	2.0
1	E	167	TYR	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
3	GOL	A	902	6/6	0.77	0.17	47,49,50,50	0
3	GOL	C	904	6/6	0.80	0.16	48,51,53,55	0
3	GOL	E	903	6/6	0.82	0.14	43,46,46,46	0
3	GOL	B	901	6/6	0.86	0.11	51,55,61,65	0
2	ZN	B	301	1/1	0.97	0.09	47,47,47,47	0
2	ZN	D	300	1/1	0.97	0.05	41,41,41,41	0
2	ZN	D	301	1/1	0.98	0.08	41,41,41,41	0
2	ZN	E	301	1/1	0.98	0.04	36,36,36,36	0
2	ZN	B	300	1/1	0.98	0.10	42,42,42,42	0
2	ZN	C	300	1/1	0.99	0.07	40,40,40,40	0
2	ZN	C	301	1/1	0.99	0.06	39,39,39,39	0
2	ZN	A	300	1/1	0.99	0.06	38,38,38,38	0
2	ZN	A	301	1/1	0.99	0.07	38,38,38,38	0
2	ZN	E	300	1/1	0.99	0.03	35,35,35,35	0
2	ZN	F	300	1/1	1.00	0.02	34,34,34,34	0
2	ZN	F	301	1/1	1.00	0.04	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.