Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 04:58 AM EST

PDB ID	:	1Q3K
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 (i) 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 (1)) were used in the production of this report:

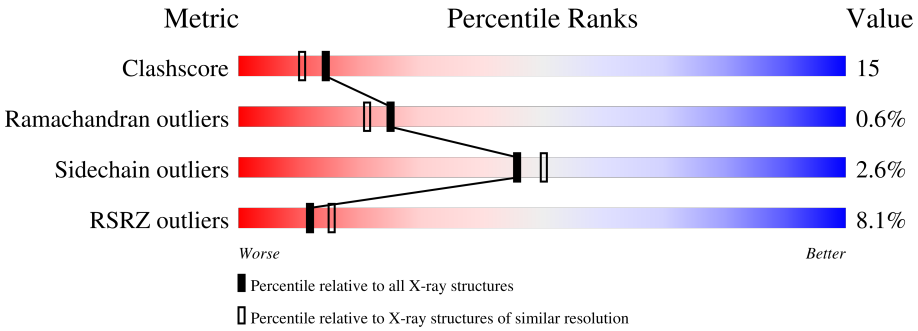
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	7% 71% 25% ·
1	B	259	9% 71% 26% ·
1	C	259	10% 68% 29% ·
1	D	259	12% 69% 29% ·
1	E	259	6% 73% 24% ·
1	F	259	5% 72% 25% ·

2 Entry composition (i)

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	C	N	O	S	0	0	0
			2000	1281	340	369	10			
1	B	259	Total	C	N	O	S	0	0	0
			2000	1281	340	369	10			
1	C	259	Total	C	N	O	S	0	0	0
			2000	1281	340	369	10			
1	D	259	Total	C	N	O	S	0	0	0
			2000	1281	340	369	10			
1	E	259	Total	C	N	O	S	0	0	0
			2000	1281	340	369	10			
1	F	259	Total	C	N	O	S	0	0	0
			2000	1281	340	369	10			

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

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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 (three-letter code: 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

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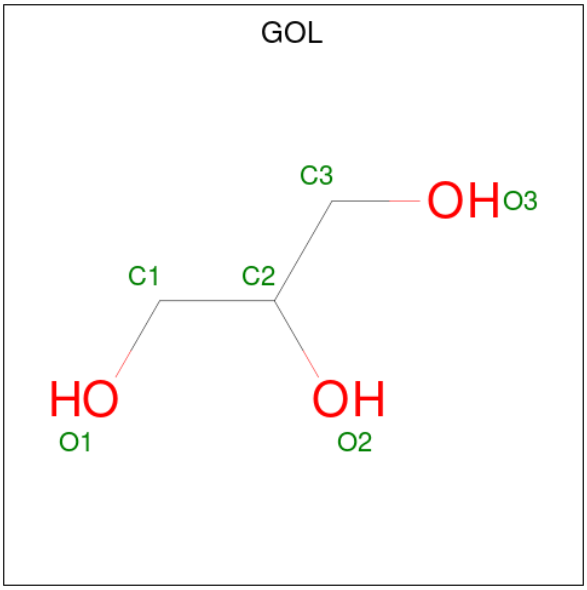
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

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

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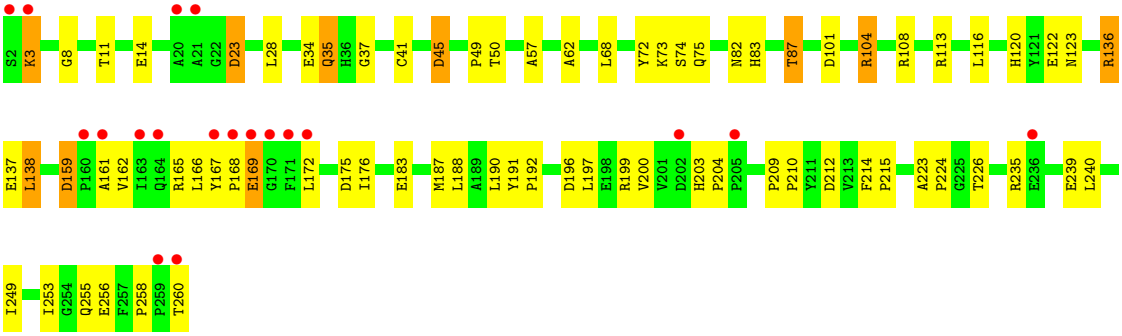
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	113	Total O 113 113	0	0
4	E	125	Total O 125 125	0	0
4	F	134	Total O 134 134	0	0

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.

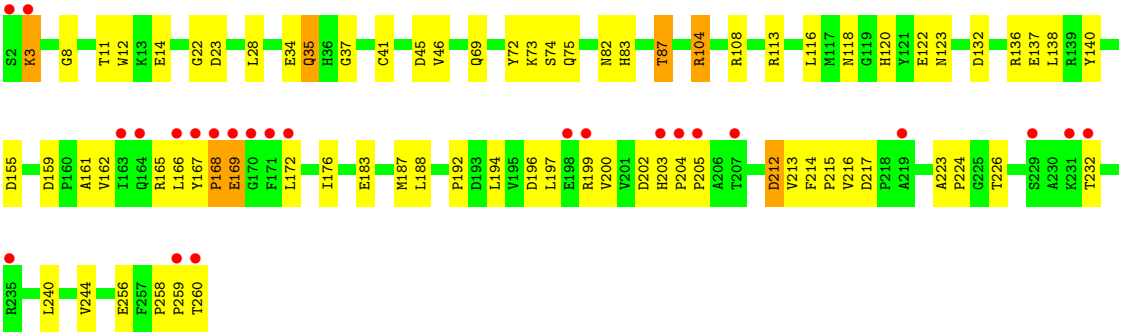
• Molecule 1: creatininase

Chain A:



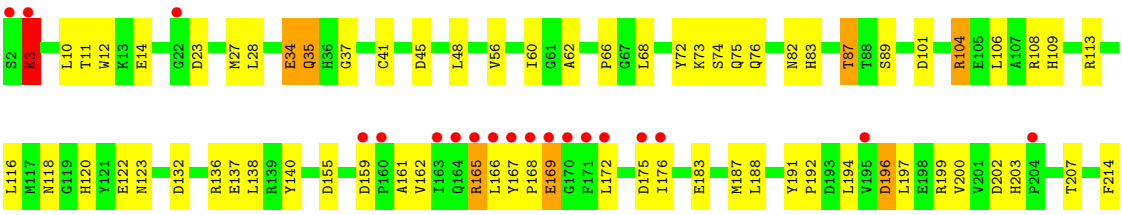
• Molecule 1: creatininase

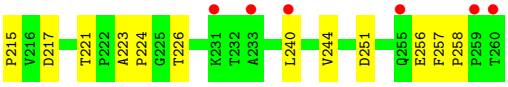
Chain B:



• Molecule 1: creatininase

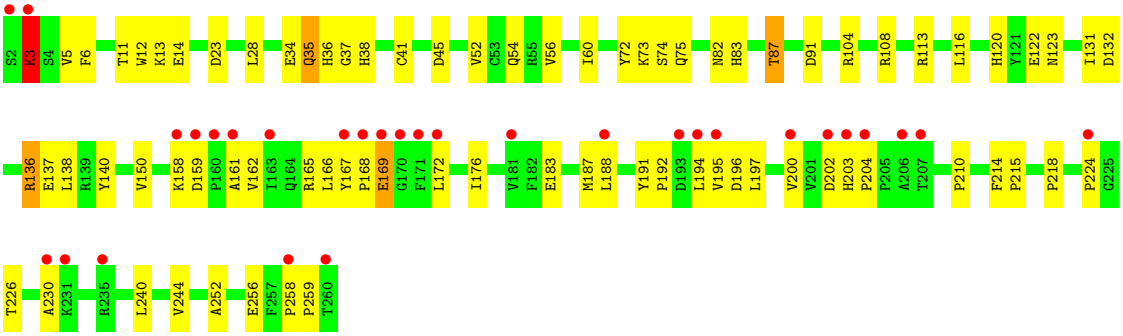
Chain C:





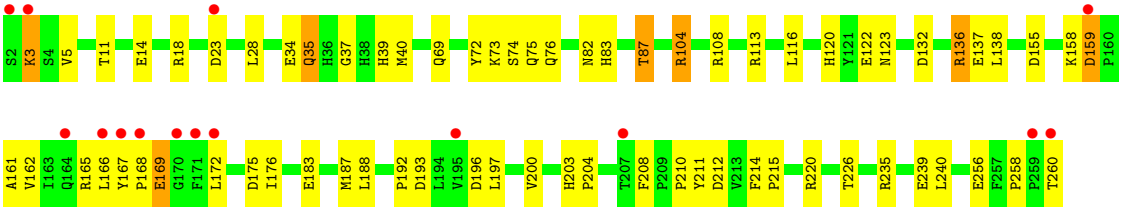
• Molecule 1: creatininase

Chain D:



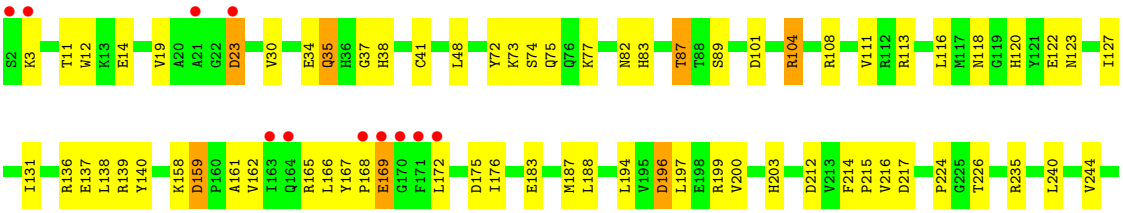
• Molecule 1: creatininase

Chain E:



• Molecule 1: creatininase

Chain F:



4 Data and refinement statistics (i)

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 29.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	79.5 (50.00-2.10) 79.5 (29.98-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [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 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.92	0/2050	0.86	7/2792 (0.3%)
1	B	0.94	0/2050	0.89	9/2792 (0.3%)
1	C	0.96	1/2050 (0.0%)	0.93	11/2792 (0.4%)
1	D	0.92	0/2050	0.89	7/2792 (0.3%)
1	E	0.91	0/2050	0.91	9/2792 (0.3%)
1	F	0.94	0/2050	0.87	7/2792 (0.3%)
All	All	0.93	1/12300 (0.0%)	0.89	50/16752 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	34	GLU	CD-OE1	5.18	1.31	1.25

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	104	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	E	136	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	C	104	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	45	ASP	CB-CG-OD2	8.37	125.83	118.30
1	E	132	ASP	CB-CG-OD2	8.35	125.81	118.30
1	D	136	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	A	45	ASP	CB-CG-OD2	8.00	125.50	118.30
1	A	104	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	E	136	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	B	132	ASP	CB-CG-OD2	7.60	125.14	118.30
1	D	196	ASP	CB-CG-OD2	7.38	124.94	118.30
1	C	132	ASP	CB-CG-OD2	7.30	124.87	118.30
1	D	45	ASP	CB-CG-OD2	7.21	124.79	118.30
1	C	45	ASP	CB-CG-OD2	7.18	124.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	104	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	F	104	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	C	202	ASP	CB-CG-OD2	7.03	124.63	118.30
1	E	175	ASP	CB-CG-OD2	6.89	124.50	118.30
1	B	202	ASP	CB-CG-OD2	6.44	124.10	118.30
1	B	136	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	E	155	ASP	CB-CG-OD2	6.38	124.04	118.30
1	C	217	ASP	CB-CG-OD1	6.31	123.98	118.30
1	C	251	ASP	CB-CG-OD2	6.28	123.96	118.30
1	D	136	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	104	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	D	91	ASP	CB-CG-OD2	6.09	123.78	118.30
1	C	155	ASP	CB-CG-OD2	6.04	123.74	118.30
1	D	202	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	104	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	104	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	136	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	F	23	ASP	CB-CG-OD2	5.76	123.49	118.30
1	F	175	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	23	ASP	CB-CG-OD2	5.75	123.47	118.30
1	D	132	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	175	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	196	ASP	CB-CG-OD2	5.58	123.33	118.30
1	E	196	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	155	ASP	CB-CG-OD1	5.52	123.27	118.30
1	E	104	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	212	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	159	ASP	CB-CG-OD2	5.35	123.11	118.30
1	C	136	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	136	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	F	196	ASP	CB-CG-OD2	5.25	123.02	118.30
1	F	217	ASP	CB-CG-OD2	5.24	123.02	118.30
1	E	193	ASP	CB-CG-OD2	5.15	122.94	118.30
1	F	159	ASP	CB-CG-OD2	5.13	122.92	118.30
1	E	159	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	175	ASP	CB-CG-OD2	5.02	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	67	0
1	B	2000	0	1980	64	0
1	C	2000	0	1980	70	0
1	D	2000	0	1980	71	0
1	E	2000	0	1980	54	0
1	F	2000	0	1980	63	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
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	10	0
4	D	113	0	0	15	1
4	E	125	0	0	9	0
4	F	134	0	0	12	1
All	All	12760	0	11912	371	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 15.

All (371) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:ARG:HD3	4:F:389:HOH:O	1.66	0.95
1:B:3:LYS:NZ	1:B:3:LYS:HA	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: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
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:3:LYS:HA	1:B:3:LYS:HZ3	1.53	0.72
1:B:216:VAL:HA	4:B:969:HOH:O	1.88	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:C:3:LYS:HA	1:C:3:LYS:HZ2	1.54	0.71
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:B:3:LYS:HA	1:B:3:LYS:HZ2	1.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:PHE:HA	1:D:215:PRO:C	2.14	0.67
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: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
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: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:A:188:LEU:C	4:A:1012:HOH:O	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:214:PHE:HA	1:C:215:PRO:C	2.23	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: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
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:6:PHE:HE1	1:D:54:GLN:NE2	2.02	0.57
1:E:256:GLU:C	1:E:258:PRO:HD3	2.25	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: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: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:B:256:GLU:C	1:B:258:PRO:HD3	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:256:GLU:C	1:C:258:PRO:HD3	2.27	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:F:256:GLU:C	1:F:258:PRO:HD3	2.28	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
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:D:256:GLU:C	1:D:258:PRO:HD3	2.29	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:B:197:LEU:HD13	1:B:200:VAL:HG21	1.90	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:E:120:HIS:HA	4:E:905:HOH:O	2.09	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:E:214:PHE:HA	1:E:215:PRO:C	2.30	0.52
1:F:120:HIS:HB3	1:F:123:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLU:C	1:A:258:PRO:HD3	2.31	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:D:52:VAL:O	1:D:56:VAL:HG23	2.11	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:A:168:PRO:O	1:A:169:GLU:HB2	2.11	0.51
1:F:240:LEU:O	1:F:244:VAL:HG23	2.11	0.51
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: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:F:214:PHE:HA	1:F:215:PRO:C	2.32	0.50
1:A:87:THR:HG21	4:A:906:HOH:O	2.12	0.50
1:C:10:LEU:O	1:D:41:CYS:HA	2.12	0.50
1:C:166:LEU:C	1:C:168:PRO:HD3	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:166:LEU:C	1:B:168:PRO:HD3	2.33	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:F:166:LEU:C	1:F:168:PRO:HD3	2.33	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:A:166:LEU:C	1:A:168:PRO:HD3	2.35	0.47
1:A:214:PHE:HA	1:A:215:PRO:C	2.33	0.47
1:B:214:PHE:HA	1:B:215:PRO:C	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:E:166:LEU:C	1:E:168:PRO:HD3	2.35	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3:LYS:HA	1:C:3:LYS:HZ3	1.76	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: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: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: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:D:214:PHE:CA	1:D:215:PRO:C	2.85	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:166:LEU:C	1:D:168:PRO:HD3	2.39	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:77:LYS:NZ	4:F:427:HOH:O	2.53	0.41
1:A:188:LEU:O	1:A:192:PRO:HG3	2.21	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%)	34	32
1	B	257/259 (99%)	242 (94%)	13 (5%)	2 (1%)	19	15
1	C	257/259 (99%)	241 (94%)	14 (5%)	2 (1%)	19	15
1	D	257/259 (99%)	243 (95%)	12 (5%)	2 (1%)	19	15
1	E	257/259 (99%)	244 (95%)	12 (5%)	1 (0%)	34	32
1	F	257/259 (99%)	243 (95%)	13 (5%)	1 (0%)	34	32
All	All	1542/1554 (99%)	1456 (94%)	77 (5%)	9 (1%)	25	21

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%)	208 (97%)	6 (3%)	43 47
1	B	214/214 (100%)	208 (97%)	6 (3%)	43 47
1	C	214/214 (100%)	209 (98%)	5 (2%)	50 55
1	D	214/214 (100%)	209 (98%)	5 (2%)	50 55
1	E	214/214 (100%)	208 (97%)	6 (3%)	43 47
1	F	214/214 (100%)	209 (98%)	5 (2%)	50 55
All	All	1284/1284 (100%)	1251 (97%)	33 (3%)	46 50

All (33) 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	212	ASP
1	B	3	LYS
1	B	35	GLN
1	B	87	THR
1	B	138	LEU
1	B	165	ARG
1	B	212	ASP
1	C	3	LYS
1	C	35	GLN
1	C	87	THR
1	C	138	LEU
1	C	165	ARG
1	D	3	LYS
1	D	35	GLN
1	D	87	THR
1	D	138	LEU
1	D	165	ARG
1	E	3	LYS
1	E	35	GLN
1	E	87	THR
1	E	138	LEU
1	E	165	ARG

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Mol	Chain	Res	Type
1	E	212	ASP
1	F	35	GLN
1	F	87	THR
1	F	138	LEU
1	F	165	ARG
1	F	212	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) 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	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	75	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
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	82	ASN
1	E	83	HIS
1	E	118	ASN
1	E	203	HIS

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Mol	Chain	Res	Type
1	E	255	GLN
1	F	35	GLN
1	F	75	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 monosaccharides 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	C	904	-	5,5,5	0.43	0	5,5,5	0.51	0
3	GOL	E	903	-	5,5,5	0.44	0	5,5,5	0.46	0
3	GOL	B	901	-	5,5,5	0.32	0	5,5,5	0.53	0
3	GOL	A	902	-	5,5,5	0.71	0	5,5,5	0.91	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	C	904	-	-	0/4/4/4	-
3	GOL	E	903	-	-	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	C	904	GOL	1	0
3	E	903	GOL	1	0
3	B	901	GOL	2	0
3	A	902	GOL	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^{th} 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%)	0.42	19 (7%) 15 19	22, 40, 68, 85	0
1	B	259/259 (100%)	0.48	24 (9%) 8 11	23, 40, 68, 85	0
1	C	259/259 (100%)	0.49	25 (9%) 7 10	22, 40, 68, 86	0
1	D	259/259 (100%)	0.51	30 (11%) 4 6	21, 39, 68, 86	0
1	E	259/259 (100%)	0.28	15 (5%) 23 28	21, 38, 68, 85	0
1	F	259/259 (100%)	0.26	13 (5%) 28 34	20, 38, 67, 85	0
All	All	1554/1554 (100%)	0.41	126 (8%) 12 15	20, 39, 68, 86	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	10.9
1	E	2	SER	9.8
1	C	2	SER	9.0
1	F	2	SER	7.9
1	C	170	GLY	7.1
1	C	168	PRO	6.7
1	B	166	LEU	6.5
1	A	21	ALA	6.4
1	A	260	THR	6.3
1	D	171	PHE	6.2
1	B	171	PHE	6.0
1	D	2	SER	5.7
1	B	167	TYR	5.7
1	B	170	GLY	5.6
1	B	2	SER	5.5
1	F	260	THR	5.4
1	B	169	GLU	5.2
1	C	167	TYR	5.2
1	B	172	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	172	LEU	5.1
1	D	170	GLY	5.1
1	E	172	LEU	5.1
1	F	170	GLY	5.1
1	C	171	PHE	5.1
1	E	3	LYS	4.8
1	F	171	PHE	4.7
1	E	170	GLY	4.6
1	E	260	THR	4.5
1	D	3	LYS	4.5
1	D	169	GLU	4.5
1	A	160	PRO	4.5
1	A	170	GLY	4.5
1	C	169	GLU	4.5
1	D	172	LEU	4.4
1	A	259	PRO	4.3
1	C	172	LEU	4.1
1	D	195	VAL	4.0
1	C	22	GLY	4.0
1	D	159	ASP	3.9
1	F	172	LEU	3.9
1	C	260	THR	3.8
1	A	164	GLN	3.8
1	D	224	PRO	3.8
1	D	194	LEU	3.8
1	C	259	PRO	3.7
1	A	171	PHE	3.7
1	B	198	GLU	3.7
1	D	167	TYR	3.6
1	A	161	ALA	3.6
1	A	205	PRO	3.6
1	E	168	PRO	3.6
1	E	164	GLN	3.4
1	B	3	LYS	3.4
1	B	168	PRO	3.4
1	E	171	PHE	3.4
1	B	205	PRO	3.4
1	C	163	ILE	3.3
1	B	164	GLN	3.2
1	C	3	LYS	3.1
1	B	163	ILE	3.1
1	E	23	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	168	PRO	3.0
1	F	21	ALA	3.0
1	B	229	SER	3.0
1	D	200	VAL	3.0
1	B	204	PRO	3.0
1	C	164	GLN	2.8
1	F	168	PRO	2.8
1	F	259	PRO	2.8
1	D	163	ILE	2.8
1	C	240	LEU	2.8
1	E	159	ASP	2.7
1	A	202	ASP	2.7
1	B	260	THR	2.7
1	D	188	LEU	2.6
1	B	235	ARG	2.6
1	C	231	LYS	2.6
1	D	193	ASP	2.6
1	A	169	GLU	2.6
1	E	207	THR	2.6
1	D	258	PRO	2.6
1	D	230	ALA	2.6
1	D	160	PRO	2.6
1	C	166	LEU	2.6
1	C	195	VAL	2.5
1	B	231	LYS	2.5
1	B	232	THR	2.5
1	A	3	LYS	2.4
1	D	231	LYS	2.4
1	E	195	VAL	2.4
1	A	20	ALA	2.4
1	D	203	HIS	2.4
1	D	181	VAL	2.3
1	F	169	GLU	2.3
1	C	255	GLN	2.3
1	A	236	GLU	2.3
1	D	202	ASP	2.3
1	B	207	THR	2.3
1	F	3	LYS	2.3
1	B	259	PRO	2.3
1	D	260	THR	2.3
1	F	164	GLN	2.2
1	D	235	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	163	ILE	2.2
1	A	168	PRO	2.2
1	E	166	LEU	2.2
1	C	159	ASP	2.2
1	D	158	LYS	2.2
1	E	259	PRO	2.2
1	A	163	ILE	2.1
1	C	176	ILE	2.1
1	F	23	ASP	2.1
1	C	204	PRO	2.1
1	C	165	ARG	2.1
1	D	161	ALA	2.1
1	C	175	ASP	2.1
1	C	160	PRO	2.1
1	D	204	PRO	2.1
1	B	199	ARG	2.1
1	B	203	HIS	2.1
1	D	206	ALA	2.0
1	E	167	TYR	2.0
1	B	219	ALA	2.0
1	C	233	ALA	2.0
1	A	167	TYR	2.0
1	D	207	THR	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^{th} 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	E	903	6/6	0.79	0.23	43,46,46,46	0
3	GOL	C	904	6/6	0.82	0.24	48,51,53,55	0
3	GOL	A	902	6/6	0.87	0.29	47,49,50,50	0
3	GOL	B	901	6/6	0.87	0.19	51,55,61,65	0
2	ZN	D	300	1/1	0.95	0.05	41,41,41,41	0
2	ZN	B	300	1/1	0.98	0.03	42,42,42,42	0
2	ZN	D	301	1/1	0.98	0.05	41,41,41,41	0
2	ZN	B	301	1/1	0.98	0.03	47,47,47,47	0
2	ZN	E	301	1/1	0.99	0.08	36,36,36,36	0
2	ZN	F	300	1/1	0.99	0.08	34,34,34,34	0
2	ZN	C	301	1/1	0.99	0.05	39,39,39,39	0
2	ZN	A	301	1/1	0.99	0.03	38,38,38,38	0
2	ZN	C	300	1/1	0.99	0.04	40,40,40,40	0
2	ZN	E	300	1/1	0.99	0.07	35,35,35,35	0
2	ZN	A	300	1/1	1.00	0.05	38,38,38,38	0
2	ZN	F	301	1/1	1.00	0.05	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.