



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2024 – 08:31 AM EDT

PDB ID : 4ZGJ
Title : Double Mutant H80A/H81A of Fe-Type Nitrile Hydratase from *Comamonas testosteroni* Ni1
Authors : Wu, R.; Martinez, S.; Holz, R.; Liu, D.
Deposited on : 2015-04-23
Resolution : 2.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

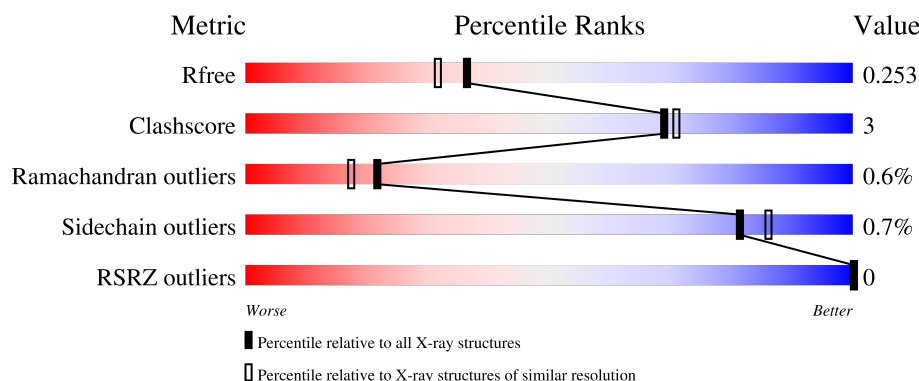
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	206	
1	C	206	
1	E	206	
1	G	206	
1	I	206	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	206	 89% 11%
1	M	206	 89% 10% •
1	O	206	 93% 7%
2	B	206	 92% 8%
2	D	206	 91% 8%
2	F	206	 91% 9%
2	H	206	 96% •
2	J	206	 89% 11%
2	L	206	 92% 7%
2	N	206	 96% •
2	P	206	 96% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30534 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 Nitrile hydratase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	3	0
			1615	1031	265	310	9			
1	C	206	Total	C	N	O	S	0	0	0
			1599	1020	264	306	9			
1	E	206	Total	C	N	O	S	0	0	0
			1599	1020	264	306	9			
1	G	206	Total	C	N	O	S	0	0	0
			1599	1020	264	306	9			
1	I	206	Total	C	N	O	S	0	1	0
			1605	1024	264	308	9			
1	K	206	Total	C	N	O	S	0	0	0
			1599	1020	264	306	9			
1	M	206	Total	C	N	O	S	0	1	0
			1605	1024	264	308	9			
1	O	206	Total	C	N	O	S	0	0	0
			1599	1020	264	306	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	ALA	HIS	engineered mutation	UNP J9PBS0
A	81	ALA	HIS	engineered mutation	UNP J9PBS0
C	80	ALA	HIS	engineered mutation	UNP J9PBS0
C	81	ALA	HIS	engineered mutation	UNP J9PBS0
E	80	ALA	HIS	engineered mutation	UNP J9PBS0
E	81	ALA	HIS	engineered mutation	UNP J9PBS0
G	80	ALA	HIS	engineered mutation	UNP J9PBS0
G	81	ALA	HIS	engineered mutation	UNP J9PBS0
I	80	ALA	HIS	engineered mutation	UNP J9PBS0
I	81	ALA	HIS	engineered mutation	UNP J9PBS0
K	80	ALA	HIS	engineered mutation	UNP J9PBS0
K	81	ALA	HIS	engineered mutation	UNP J9PBS0
M	80	ALA	HIS	engineered mutation	UNP J9PBS0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	81	ALA	HIS	engineered mutation	UNP J9PBS0
O	80	ALA	HIS	engineered mutation	UNP J9PBS0
O	81	ALA	HIS	engineered mutation	UNP J9PBS0

- Molecule 2 is a protein called Nitrile hydratase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	D	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	F	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	H	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	J	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	L	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	N	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	P	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	112	PRO	ALA	conflict	UNP J9PBS1
D	112	PRO	ALA	conflict	UNP J9PBS1
F	112	PRO	ALA	conflict	UNP J9PBS1
H	112	PRO	ALA	conflict	UNP J9PBS1
J	112	PRO	ALA	conflict	UNP J9PBS1
L	112	PRO	ALA	conflict	UNP J9PBS1
N	112	PRO	ALA	conflict	UNP J9PBS1
P	112	PRO	ALA	conflict	UNP J9PBS1

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Fe 1	0	0
3	E	1	Total 1	Fe 1	0	0
3	G	1	Total 1	Fe 1	0	0
3	I	1	Total 1	Fe 1	0	0
3	K	1	Total 1	Fe 1	0	0
3	M	1	Total 1	Fe 1	0	0
3	O	1	Total 1	Fe 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	285	Total 285	O 285	0	0
4	B	310	Total 310	O 310	0	0
4	C	325	Total 325	O 325	0	0
4	D	304	Total 304	O 304	0	0
4	E	352	Total 352	O 352	0	0
4	F	311	Total 311	O 311	0	0
4	G	332	Total 332	O 332	0	0
4	H	291	Total 291	O 291	0	0
4	I	287	Total 287	O 287	0	0
4	J	336	Total 336	O 336	0	0
4	K	352	Total 352	O 352	0	0
4	L	296	Total 296	O 296	0	0

Continued on next page...


Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	325	Total 325	O 325	0	0
4	N	323	Total 323	O 323	0	0
4	O	269	Total 269	O 269	0	0
4	P	296	Total 296	O 296	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: Nitrile hydratase alpha subunit

Chain A: 




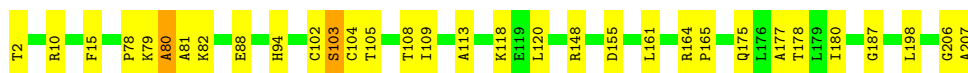
- Molecule 1: Nitrile hydratase alpha subunit

Chain C: 



- Molecule 1: Nitrile hydratase alpha subunit

Chain E: 




- Molecule 1: Nitrile hydratase alpha subunit

Chain G: 




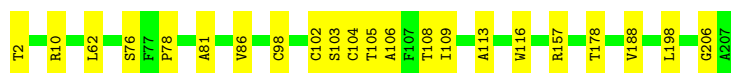
- Molecule 1: Nitrile hydratase alpha subunit

Chain I: 



- Molecule 1: Nitrile hydratase alpha subunit

Chain K: 



- Molecule 1: Nitrile hydratase alpha subunit

Chain M: 89% 10%



- Molecule 1: Nitrile hydratase alpha subunit

Chain O: 93% 7%



- Molecule 2: Nitrile hydratase beta subunit

Chain B: 92% 8%



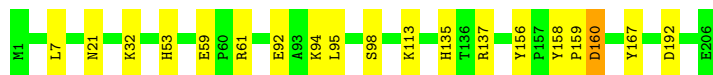
- Molecule 2: Nitrile hydratase beta subunit

Chain D: 91% 8%



- Molecule 2: Nitrile hydratase beta subunit

Chain F: 91% 9%



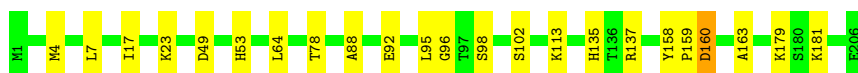
- Molecule 2: Nitrile hydratase beta subunit

Chain H: 96%



- Molecule 2: Nitrile hydratase beta subunit

Chain J: 89% 11%



- Molecule 2: Nitrile hydratase beta subunit

Chain L: 92% 7%



- Molecule 2: Nitrile hydratase beta subunit

Chain N: 96% .



- Molecule 2: Nitrile hydratase beta subunit

Chain P: 96% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	112.05Å 112.05Å 476.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.57 – 2.00 36.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.57-2.00) 98.5 (36.57-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.41	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.220 , 0.253 0.222 , 0.253	Depositor DCC
R_{free} test set	22301 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.387 for -h,-k,l 0.379 for h,-h-k,-l 0.389 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30534	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: CSD, FE

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	0.21	0/1643	0.38	0/2245
1	C	0.23	0/1618	0.43	0/2211
1	E	0.21	0/1618	0.39	0/2211
1	G	0.21	0/1618	0.40	0/2211
1	I	0.21	0/1627	0.39	0/2223
1	K	0.21	0/1618	0.39	0/2211
1	M	0.21	0/1627	0.39	0/2223
1	O	0.21	0/1618	0.38	0/2211
2	B	0.21	0/1636	0.37	0/2216
2	D	0.21	0/1636	0.38	0/2216
2	F	0.22	0/1636	0.38	0/2216
2	H	0.21	0/1636	0.38	0/2216
2	J	0.21	0/1636	0.37	0/2216
2	L	0.22	0/1636	0.38	0/2216
2	N	0.21	0/1636	0.37	0/2216
2	P	0.21	0/1636	0.37	0/2216
All	All	0.21	0/26075	0.38	0/35474

There are no bond length outliers.

There are no bond angle outliers.

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	1615	0	1607	15	1
1	C	1599	0	1586	22	0
1	E	1599	0	1586	22	0
1	G	1599	0	1586	9	0
1	I	1605	0	1592	12	0
1	K	1599	0	1586	11	0
1	M	1605	0	1592	15	0
1	O	1599	0	1586	6	0
2	B	1589	0	1534	13	0
2	D	1589	0	1534	13	0
2	F	1589	0	1534	13	0
2	H	1589	0	1534	6	0
2	J	1589	0	1534	16	0
2	L	1589	0	1534	11	0
2	N	1589	0	1534	6	0
2	P	1589	0	1534	5	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
4	A	285	0	0	4	0
4	B	310	0	0	1	0
4	C	325	0	0	5	1
4	D	304	0	0	2	0
4	E	352	0	0	3	0
4	F	311	0	0	0	0
4	G	332	0	0	2	0
4	H	291	0	0	1	0
4	I	287	0	0	3	1
4	J	336	0	0	3	0
4	K	352	0	0	2	0
4	L	296	0	0	3	0
4	M	325	0	0	5	0
4	N	323	0	0	1	0
4	O	269	0	0	0	1
4	P	296	0	0	1	0
All	All	30534	0	24993	172	2

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 3.

All (172) 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:K:98:CYS:SG	4:K:550:HOH:O	2.34	0.84
1:A:67:VAL:O	4:A:401:HOH:O	1.99	0.80
1:I:37:MET:O	4:I:401:HOH:O	2.05	0.75
1:E:81:ALA:HB2	1:E:155:ASP:HB3	1.69	0.75
1:A:71:GLU:N	4:A:401:HOH:O	2.08	0.71
2:N:18:LYS:NZ	4:N:301:HOH:O	2.23	0.70
1:M:79:LYS:NZ	4:M:404:HOH:O	2.26	0.68
1:C:102:CSD:OD1	2:D:137:ARG:NH2	2.25	0.68
2:J:4:MET:SD	4:J:563:HOH:O	2.52	0.68
1:E:10:ARG:HG2	2:F:95:LEU:HD21	1.77	0.66
1:G:10:ARG:HG2	2:H:95:LEU:HD21	1.77	0.65
1:E:2:THR:N	4:E:405:HOH:O	2.30	0.64
1:K:198:LEU:HD12	1:M:198:LEU:HD12	1.79	0.64
1:M:27:GLN:NE2	4:M:406:HOH:O	2.30	0.64
1:C:27:GLN:HE21	1:C:27:GLN:N	1.96	0.63
1:E:198:LEU:HD12	1:I:198:LEU:HD12	1.79	0.62
2:J:179:LYS:HD3	2:J:181:LYS:HE2	1.82	0.61
2:D:124:ARG:NH1	4:D:307:HOH:O	2.34	0.60
2:P:43:LYS:NZ	4:P:306:HOH:O	2.34	0.60
1:M:27:GLN:NE2	4:M:410:HOH:O	2.34	0.60
1:C:26:ASP:C	1:C:27:GLN:HE21	2.05	0.60
1:G:43:GLN:NE2	4:G:406:HOH:O	2.35	0.59
1:I:10:ARG:HG2	2:J:95:LEU:HD21	1.84	0.58
1:M:48:LEU:HD23	1:M:73:LEU:HD12	1.84	0.58
1:E:82:LYS:O	4:E:401:HOH:O	2.17	0.58
2:L:181:LYS:NZ	4:L:307:HOH:O	2.35	0.58
1:K:106:ALA:HB2	1:K:157:ARG:HB3	1.84	0.58
2:J:113:LYS:NZ	4:J:306:HOH:O	2.35	0.58
1:I:2:THR:OG1	4:I:402:HOH:O	2.17	0.57
1:G:106:ALA:HB2	1:G:157:ARG:HB3	1.86	0.57
2:P:92:GLU:HG2	2:P:98:SER:HA	1.86	0.57
2:D:23:LYS:NZ	4:D:311:HOH:O	2.38	0.56
2:D:124:ARG:HB2	2:D:206:GLU:HG2	1.86	0.56
1:E:81:ALA:HB3	1:E:82:LYS:HA	1.88	0.56
1:K:108:THR:HG23	1:K:109:ILE:HG12	1.87	0.56
1:C:27:GLN:HE21	1:C:27:GLN:CA	2.19	0.56
2:N:179:LYS:HD3	2:N:181:LYS:HE2	1.88	0.55
1:A:3:ASP:OD1	1:A:4:ASN:N	2.38	0.55
2:H:181:LYS:NZ	4:H:315:HOH:O	2.41	0.54
1:A:40:TRP:CD1	1:A:108[B]:THR:HG23	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:ARG:HD3	2:D:137:ARG:NH2	2.24	0.53
2:L:124:ARG:NH1	4:L:308:HOH:O	2.38	0.53
1:C:108:THR:HG23	1:C:109:ILE:HG12	1.90	0.53
1:C:94:HIS:O	4:C:401:HOH:O	2.18	0.52
1:E:103:SER:HB2	1:E:118:LYS:HG2	1.89	0.52
1:A:108[A]:THR:HG23	1:A:109:ILE:HG12	1.91	0.52
1:K:105:THR:HG21	1:K:113:ALA:HB2	1.91	0.52
1:C:103:SER:HB2	1:C:118:LYS:HG2	1.91	0.52
2:L:52:ARG:NH2	4:L:306:HOH:O	2.35	0.52
1:A:48:LEU:HD12	1:A:73:LEU:HD12	1.91	0.52
1:I:48:LEU:HD23	1:I:73:LEU:HD12	1.92	0.52
1:M:103:SER:HB2	1:M:118:LYS:HG2	1.91	0.52
1:E:94:HIS:NE2	1:E:187:GLY:O	2.39	0.51
1:G:108:THR:HG23	1:G:109:ILE:HG12	1.92	0.51
1:G:103:SER:HB2	1:G:118:LYS:HG2	1.91	0.51
1:A:11:VAL:HG12	2:B:32:LYS:HE3	1.93	0.51
2:H:59:GLU:OE2	2:H:61:ARG:NH1	2.43	0.51
1:M:116:TRP:CH2	1:M:188:VAL:HG21	2.46	0.51
1:C:82:LYS:NZ	4:C:404:HOH:O	2.27	0.51
1:A:116:TRP:CD1	2:B:18:LYS:HG3	2.46	0.50
1:M:21:LEU:HD23	2:N:85:VAL:HG12	1.93	0.50
2:F:92:GLU:HG2	2:F:98:SER:HA	1.93	0.50
2:B:120:LYS:NZ	4:B:307:HOH:O	2.34	0.50
1:K:10:ARG:HG2	2:L:95:LEU:HD21	1.92	0.50
1:E:105:THR:HG21	1:E:113:ALA:HB2	1.93	0.50
1:O:108:THR:HG23	1:O:109:ILE:HG12	1.94	0.50
1:A:51:LYS:NZ	4:A:411:HOH:O	2.37	0.49
2:F:158:TYR:CE2	2:F:160:ASP:HB2	2.48	0.49
1:E:120:LEU:HD22	2:F:7:LEU:HD11	1.94	0.48
1:O:116:TRP:CH2	1:O:188:VAL:HG21	2.48	0.48
1:C:48:LEU:HD12	1:C:73:LEU:HD12	1.94	0.48
2:L:78:THR:HG21	2:L:102:SER:HB2	1.94	0.48
1:A:12:ASP:OD1	2:B:32:LYS:NZ	2.32	0.48
1:E:88:GLU:HA	1:E:161:LEU:HB3	1.96	0.48
2:H:158:TYR:CE2	2:H:160:ASP:HB2	2.49	0.48
1:O:67:VAL:HG21	1:O:82:LYS:O	2.14	0.48
1:C:206:GLY:HA2	1:C:207:ALA:HA	1.51	0.48
1:K:62:LEU:HG	1:K:86:VAL:HG21	1.95	0.48
2:F:94:LYS:HB2	2:F:94:LYS:HE2	1.54	0.47
1:C:115:ASP:O	1:C:119:GLU:HG2	2.13	0.47
1:O:48:LEU:HD23	1:O:73:LEU:HD12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:ARG:HA	2:J:64:LEU:HD23	1.96	0.47
1:C:106:ALA:HB2	1:C:157:ARG:HB3	1.97	0.47
1:C:153:THR:O	2:D:137:ARG:HD2	2.15	0.46
2:J:92:GLU:HG2	2:J:98:SER:HA	1.96	0.46
2:L:92:GLU:HG2	2:L:98:SER:HA	1.96	0.46
1:I:106:ALA:HB2	1:I:157:ARG:HB3	1.97	0.46
1:C:115:ASP:OD2	1:C:116:TRP:N	2.47	0.46
1:C:129:GLN:NE2	4:C:415:HOH:O	2.43	0.46
2:D:78:THR:HG21	2:D:102:SER:HB2	1.96	0.46
1:G:206:GLY:HA2	1:G:207:ALA:HA	1.64	0.46
1:C:26:ASP:OD2	4:C:402:HOH:O	2.20	0.46
2:B:124:ARG:HB2	2:B:206:GLU:HG3	1.98	0.46
2:N:160:ASP:N	2:N:160:ASP:OD1	2.48	0.46
2:D:158:TYR:CE2	2:D:160:ASP:HB2	2.51	0.46
1:G:161:LEU:HD12	1:G:162:PRO:HD2	1.98	0.46
1:I:120:LEU:HG	4:I:484:HOH:O	2.15	0.46
1:E:108:THR:HG23	1:E:109:ILE:HG12	1.97	0.45
1:E:148:ARG:HG2	2:F:192:ASP:HB2	1.98	0.45
2:L:160:ASP:N	2:L:160:ASP:OD1	2.47	0.45
1:I:78:PRO:HG2	1:I:81:ALA:HB3	1.97	0.45
1:I:82:LYS:HG3	1:I:83:HIS:N	2.31	0.45
2:B:158:TYR:CE2	2:B:160:ASP:HB2	2.51	0.45
2:B:92:GLU:HG2	2:B:98:SER:HA	1.99	0.45
2:B:158:TYR:HA	2:B:159:PRO:HD3	1.83	0.45
1:E:78:PRO:C	1:E:80:ALA:H	2.19	0.45
1:I:88:GLU:HA	1:I:161:LEU:HB3	1.99	0.45
1:M:120:LEU:HD22	2:N:7:LEU:HD11	1.99	0.45
1:M:110:ILE:HG22	1:M:185:LEU:HD13	1.99	0.44
1:O:106:ALA:HB2	1:O:157:ARG:HB3	1.99	0.44
2:L:137:ARG:HA	2:L:137:ARG:HD2	1.85	0.44
2:J:160:ASP:N	2:J:160:ASP:OD1	2.51	0.44
2:B:185:PRO:HD2	2:L:131:PHE:CE2	2.53	0.44
2:D:92:GLU:HG2	2:D:98:SER:HA	1.98	0.44
1:A:70:SER:N	4:A:401:HOH:O	2.51	0.44
1:I:120:LEU:HD22	2:J:7:LEU:HD11	2.00	0.44
1:M:164:ARG:HA	1:M:165:PRO:HD3	1.83	0.43
2:P:160:ASP:N	2:P:160:ASP:OD1	2.51	0.43
1:A:120:LEU:HD22	2:B:7:LEU:HD11	2.00	0.43
1:A:132:THR:OG1	2:B:189:GLU:OE1	2.26	0.43
2:J:95:LEU:HG	2:J:96:GLY:H	1.84	0.43
1:K:116:TRP:CH2	1:K:188:VAL:HG21	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:59:GLU:OE2	2:F:61:ARG:NH1	2.52	0.43
2:D:184:TRP:HB2	2:D:188:CYS:HB3	1.99	0.43
2:B:198:PHE:HB2	2:B:201:TYR:CE2	2.54	0.43
2:J:78:THR:HG21	2:J:102:SER:HB2	2.01	0.43
2:D:53:HIS:CG	2:D:135:HIS:HB2	2.53	0.42
2:F:137:ARG:HA	2:F:137:ARG:HD2	1.71	0.42
2:D:53:HIS:O	2:D:57:ARG:HG2	2.20	0.42
2:F:113:LYS:H	2:F:113:LYS:HG2	1.49	0.42
1:E:164:ARG:HA	1:E:165:PRO:HD3	1.89	0.42
2:N:92:GLU:HG2	2:N:98:SER:HA	2.00	0.42
1:E:15:PHE:CG	2:F:32:LYS:HE2	2.55	0.42
2:L:53:HIS:CG	2:L:135:HIS:HB2	2.55	0.42
1:C:175:GLN:O	1:C:178:THR:HG22	2.20	0.42
1:E:177:ALA:HA	1:E:180:ILE:HD12	2.02	0.42
1:G:204:ALA:O	1:G:205:LEU:HB2	2.20	0.42
1:M:115:ASP:OD2	1:M:116:TRP:N	2.53	0.42
1:E:155:ASP:HB2	2:F:156:TYR:CD2	2.55	0.42
2:F:158:TYR:HA	2:F:159:PRO:HD3	1.82	0.42
2:B:49:ASP:HB3	2:B:163:ALA:HB2	2.02	0.41
1:E:78:PRO:O	1:E:80:ALA:N	2.50	0.41
1:E:206:GLY:HA2	1:E:207:ALA:HA	1.69	0.41
1:G:2:THR:N	4:G:417:HOH:O	2.53	0.41
1:C:204:ALA:O	1:C:205:LEU:HB3	2.20	0.41
1:K:2:THR:N	4:K:425:HOH:O	2.53	0.41
2:H:78:THR:HG21	2:H:102:SER:HB2	2.02	0.41
2:J:49:ASP:HB3	2:J:163:ALA:HB2	2.03	0.41
2:L:158:TYR:HA	2:L:159:PRO:HD3	1.83	0.41
1:O:10:ARG:HG2	2:P:95:LEU:HD21	2.01	0.41
1:C:88:GLU:HA	1:C:161:LEU:HB3	2.02	0.41
2:H:158:TYR:HA	2:H:159:PRO:HD3	1.81	0.41
1:A:103:SER:HB2	1:A:118:LYS:HG2	2.02	0.41
1:I:55:ASP:HA	1:I:56:PRO:HD2	1.93	0.41
2:J:88:ALA:O	2:J:92:GLU:HG3	2.20	0.41
2:J:158:TYR:HA	2:J:159:PRO:HD3	1.82	0.41
1:K:78:PRO:HD2	1:K:81:ALA:HB3	2.03	0.41
1:A:106:ALA:HB2	1:A:157:ARG:HB3	2.03	0.41
1:E:175:GLN:O	1:E:178:THR:HG22	2.21	0.41
1:C:204:ALA:O	4:C:403:HOH:O	2.22	0.40
2:J:53:HIS:CG	2:J:135:HIS:HB2	2.56	0.40
2:J:137:ARG:HA	2:J:137:ARG:HD2	1.92	0.40
1:M:106:ALA:HB2	1:M:157:ARG:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:THR:HG21	1:C:113:ALA:HB2	2.02	0.40
1:C:116:TRP:CH2	1:C:188:VAL:HG21	2.56	0.40
1:M:148:ARG:NH2	4:M:415:HOH:O	2.41	0.40
1:E:10:ARG:NH1	4:E:414:HOH:O	2.41	0.40
2:F:53:HIS:CG	2:F:135:HIS:HB2	2.56	0.40
2:J:17:ILE:HB	4:J:309:HOH:O	2.21	0.40
1:K:76:SER:O	1:K:108:THR:OG1	2.29	0.40
1:M:108:THR:HG22	4:M:596:HOH:O	2.21	0.40
2:P:49:ASP:HB3	2:P:163:ALA:HB2	2.04	0.40

All (2) 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:C:430:HOH:O	4:O:412:HOH:O[2_555]	2.04	0.16
1:A:37:MET:O	4:I:401:HOH:O[1_655]	2.13	0.07

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	205/206 (100%)	199 (97%)	5 (2%)	1 (0%)	25	21
1	C	202/206 (98%)	194 (96%)	5 (2%)	3 (2%)	8	4
1	E	202/206 (98%)	193 (96%)	6 (3%)	3 (2%)	8	4
1	G	202/206 (98%)	189 (94%)	10 (5%)	3 (2%)	8	4
1	I	203/206 (98%)	196 (97%)	6 (3%)	1 (0%)	25	21
1	K	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	13	8
1	M	203/206 (98%)	195 (96%)	6 (3%)	2 (1%)	13	8
1	O	202/206 (98%)	197 (98%)	4 (2%)	1 (0%)	25	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	204/206 (99%)	201 (98%)	3 (2%)	0	100	100
2	D	204/206 (99%)	198 (97%)	6 (3%)	0	100	100
2	F	204/206 (99%)	197 (97%)	6 (3%)	1 (0%)	25	21
2	H	204/206 (99%)	197 (97%)	7 (3%)	0	100	100
2	J	204/206 (99%)	200 (98%)	3 (2%)	1 (0%)	25	21
2	L	204/206 (99%)	198 (97%)	5 (2%)	1 (0%)	25	21
2	N	204/206 (99%)	199 (98%)	4 (2%)	1 (0%)	25	21
2	P	204/206 (99%)	198 (97%)	5 (2%)	1 (0%)	25	21
All	All	3253/3296 (99%)	3144 (97%)	88 (3%)	21 (1%)	22	17

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	79	LYS
1	K	206	GLY
1	A	103	SER
1	C	80	ALA
1	C	103	SER
1	E	103	SER
1	G	83	HIS
1	K	103	SER
1	M	83	HIS
1	M	103	SER
1	O	103	SER
2	F	21	ASN
1	G	103	SER
1	I	103	SER
2	N	23	LYS
2	P	23	LYS
1	E	80	ALA
1	G	82	LYS
2	J	23	LYS
1	C	205	LEU
2	L	8	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	173/170 (102%)	173 (100%)	0	100	100
1	C	170/170 (100%)	167 (98%)	3 (2%)	54	59
1	E	170/170 (100%)	170 (100%)	0	100	100
1	G	170/170 (100%)	170 (100%)	0	100	100
1	I	171/170 (101%)	170 (99%)	1 (1%)	84	88
1	K	170/170 (100%)	169 (99%)	1 (1%)	84	88
1	M	171/170 (101%)	170 (99%)	1 (1%)	84	88
1	O	170/170 (100%)	169 (99%)	1 (1%)	84	88
2	B	164/165 (99%)	163 (99%)	1 (1%)	84	88
2	D	164/165 (99%)	162 (99%)	2 (1%)	67	73
2	F	164/165 (99%)	162 (99%)	2 (1%)	67	73
2	H	164/165 (99%)	163 (99%)	1 (1%)	84	88
2	J	164/165 (99%)	163 (99%)	1 (1%)	84	88
2	L	164/165 (99%)	163 (99%)	1 (1%)	84	88
2	N	164/165 (99%)	163 (99%)	1 (1%)	84	88
2	P	164/165 (99%)	162 (99%)	2 (1%)	67	73
All	All	2677/2680 (100%)	2659 (99%)	18 (1%)	81	86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	160	ASP
1	C	27	GLN
1	C	188	VAL
1	C	203	VAL
2	D	150	VAL
2	D	160	ASP
2	F	160	ASP
2	F	167	TYR
2	H	160	ASP
1	I	188	VAL
2	J	160	ASP
1	K	178	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	160	ASP
1	M	27	GLN
2	N	160	ASP
1	O	79	LYS
2	P	19	THR
2	P	160	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	27	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

16 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSD	A	102	3,1	4,7,8	0.74	0	1,8,10	2.10	1 (100%)
1	CSD	K	104	3,1	4,7,8	0.79	0	1,8,10	2.59	1 (100%)
1	CSD	C	102	3,1	4,7,8	0.84	0	1,8,10	2.44	1 (100%)
1	CSD	E	104	3,1	4,7,8	0.81	0	1,8,10	2.70	1 (100%)
1	CSD	M	102	3,1	4,7,8	0.80	0	1,8,10	2.52	1 (100%)
1	CSD	K	102	3,1	4,7,8	0.89	0	1,8,10	2.70	1 (100%)
1	CSD	A	104	3,1	4,7,8	0.83	0	1,8,10	1.44	0
1	CSD	G	102	3,1	4,7,8	0.85	0	1,8,10	2.89	1 (100%)
1	CSD	I	104	3,1	4,7,8	0.85	0	1,8,10	1.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	E	102	3,1	4,7,8	0.81	0	1,8,10	2.78	1 (100%)
1	CSD	I	102	3,1	4,7,8	0.75	0	1,8,10	1.60	0
1	CSD	O	104	3,1	4,7,8	0.82	0	1,8,10	1.74	0
1	CSD	M	104	3,1	4,7,8	0.79	0	1,8,10	2.50	1 (100%)
1	CSD	C	104	3,1	4,7,8	0.80	0	1,8,10	1.84	0
1	CSD	O	102	3,1	4,7,8	0.80	0	1,8,10	2.90	1 (100%)
1	CSD	G	104	3,1	4,7,8	0.81	0	1,8,10	1.75	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
1	CSD	A	102	3,1	-	2/2/6/8	-
1	CSD	K	104	3,1	-	1/2/6/8	-
1	CSD	C	102	3,1	-	0/2/6/8	-
1	CSD	E	104	3,1	-	1/2/6/8	-
1	CSD	M	102	3,1	-	0/2/6/8	-
1	CSD	K	102	3,1	-	0/2/6/8	-
1	CSD	A	104	3,1	-	0/2/6/8	-
1	CSD	G	102	3,1	-	1/2/6/8	-
1	CSD	I	104	3,1	-	0/2/6/8	-
1	CSD	E	102	3,1	-	1/2/6/8	-
1	CSD	I	102	3,1	-	2/2/6/8	-
1	CSD	O	104	3,1	-	0/2/6/8	-
1	CSD	M	104	3,1	-	1/2/6/8	-
1	CSD	C	104	3,1	-	0/2/6/8	-
1	CSD	O	102	3,1	-	1/2/6/8	-
1	CSD	G	104	3,1	-	0/2/6/8	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	102	CSD	OD1-SG-CB	2.90	110.95	105.60
1	G	102	CSD	OD1-SG-CB	2.89	110.93	105.60
1	E	102	CSD	OD1-SG-CB	2.78	110.72	105.60
1	E	104	CSD	OD1-SG-CB	2.70	110.58	105.60
1	K	102	CSD	OD1-SG-CB	2.70	110.57	105.60
1	K	104	CSD	OD1-SG-CB	2.59	110.38	105.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	M	102	CSD	OD1-SG-CB	2.52	110.24	105.60
1	M	104	CSD	OD1-SG-CB	2.50	110.21	105.60
1	C	102	CSD	OD1-SG-CB	2.44	110.11	105.60
1	A	102	CSD	OD1-SG-CB	2.10	109.47	105.60

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	102	CSD	CA-CB-SG-OD1
1	E	104	CSD	CA-CB-SG-OD1
1	I	102	CSD	CA-CB-SG-OD1
1	K	104	CSD	CA-CB-SG-OD1
1	M	104	CSD	CA-CB-SG-OD1
1	A	102	CSD	N-CA-CB-SG
1	E	102	CSD	N-CA-CB-SG
1	G	102	CSD	N-CA-CB-SG
1	I	102	CSD	N-CA-CB-SG
1	O	102	CSD	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	102	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	204/206 (99%)	-1.84	0 100 100	17, 28, 46, 61	3 (1%)
1	C	204/206 (99%)	-1.83	0 100 100	15, 27, 51, 66	0
1	E	204/206 (99%)	-1.82	0 100 100	16, 27, 48, 63	0
1	G	204/206 (99%)	-1.82	0 100 100	15, 27, 50, 82	0
1	I	204/206 (99%)	-1.85	0 100 100	17, 28, 43, 56	1 (0%)
1	K	204/206 (99%)	-1.83	0 100 100	15, 26, 49, 69	0
1	M	204/206 (99%)	-1.84	0 100 100	16, 27, 48, 63	1 (0%)
1	O	204/206 (99%)	-1.83	0 100 100	16, 27, 46, 66	0
2	B	206/206 (100%)	-1.83	0 100 100	17, 28, 50, 72	0
2	D	206/206 (100%)	-1.83	0 100 100	16, 27, 49, 64	0
2	F	206/206 (100%)	-1.82	0 100 100	17, 27, 50, 64	0
2	H	206/206 (100%)	-1.84	0 100 100	17, 27, 51, 66	0
2	J	206/206 (100%)	-1.83	0 100 100	17, 27, 53, 70	0
2	L	206/206 (100%)	-1.84	0 100 100	17, 26, 50, 61	0
2	N	206/206 (100%)	-1.83	0 100 100	18, 27, 48, 66	0
2	P	206/206 (100%)	-1.83	0 100 100	17, 27, 50, 66	0
All	All	3280/3296 (99%)	-1.83	0 100 100	15, 27, 50, 82	5 (0%)

There are no RSRZ outliers to report.

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

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(\AA^2)	Q<0.9
1	CSD	A	102	8/9	1.00	0.02	14,18,21,21	0
1	CSD	A	104	8/9	1.00	0.02	16,21,26,27	0
1	CSD	C	102	8/9	1.00	0.03	18,20,26,28	0
1	CSD	C	104	8/9	1.00	0.03	19,22,24,26	0
1	CSD	E	102	8/9	1.00	0.02	17,22,23,24	0
1	CSD	E	104	8/9	1.00	0.02	16,20,22,22	0
1	CSD	G	102	8/9	1.00	0.02	19,20,23,29	0
1	CSD	G	104	8/9	1.00	0.02	18,22,25,25	0
1	CSD	I	102	8/9	1.00	0.02	15,20,21,22	0
1	CSD	I	104	8/9	1.00	0.02	20,22,25,26	0
1	CSD	K	102	8/9	1.00	0.03	17,22,25,25	0
1	CSD	K	104	8/9	1.00	0.03	19,23,25,26	0
1	CSD	M	102	8/9	1.00	0.02	14,19,21,23	0
1	CSD	M	104	8/9	1.00	0.02	14,20,20,23	8
1	CSD	O	102	8/9	1.00	0.02	16,16,24,26	0
1	CSD	O	104	8/9	1.00	0.02	17,21,23,23	0

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, 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(\AA^2)	Q<0.9
3	FE	A	301	1/1	1.00	0.01	24,24,24,24	0
3	FE	C	301	1/1	1.00	0.01	24,24,24,24	0
3	FE	E	301	1/1	1.00	0.01	20,20,20,20	0
3	FE	G	301	1/1	1.00	0.01	24,24,24,24	0
3	FE	I	301	1/1	1.00	0.01	22,22,22,22	0
3	FE	K	301	1/1	1.00	0.01	22,22,22,22	0
3	FE	M	301	1/1	1.00	0.01	24,24,24,24	0
3	FE	O	301	1/1	1.00	0.01	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.