



# Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 05:24 PM GMT

PDB ID : 4OQ5  
Title : Crystal Structure of Human MCL-1 Bound to Inhibitor 4-(4-methylnaphthalen-1-yl)-2-{[(4-phenoxyphenyl)sulfonyl]amino}benzoicacid  
Authors : Petros, A.M.; Swann, S.L.; Song, D.; Swinger, K.; Park, C.; Zhang, H.; Wendt, M.D.; Kunzer, A.R.; Souers, A.J.; Sun, C.  
Deposited on : 2014-02-07  
Resolution : 2.86 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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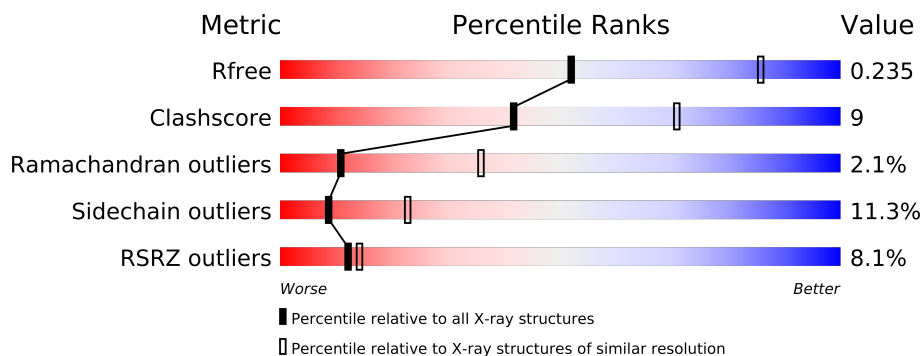
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : trunk22714  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk22714

# 1 Overall quality at a glance

The reported resolution of this entry is 2.86 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))
$R_{free}$	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	163	
1	B	163	
1	C	163	
1	D	163	
1	E	163	
1	F	163	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7736 atoms, of which 120 are hydrogens and 0 are deuterium.

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 Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1208	758	223	222	5			
1	B	151	Total	C	N	O	S	0	0	0
			1216	764	224	223	5			
1	C	149	Total	C	N	O	S	0	0	0
			1200	754	222	219	5			
1	D	149	Total	C	N	O	S	0	0	0
			1200	754	222	219	5			
1	E	151	Total	C	N	O	S	0	0	0
			1216	764	224	223	5			
1	F	149	Total	C	N	O	S	0	0	0
			1200	754	222	219	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	EXPRESSION TAG	UNP Q07820
A	165	THR	-	EXPRESSION TAG	UNP Q07820
A	166	LEU	-	EXPRESSION TAG	UNP Q07820
A	167	VAL	-	EXPRESSION TAG	UNP Q07820
A	168	PRO	-	EXPRESSION TAG	UNP Q07820
A	169	ARG	-	EXPRESSION TAG	UNP Q07820
A	170	GLY	-	EXPRESSION TAG	UNP Q07820
A	171	SER	-	EXPRESSION TAG	UNP Q07820
A	172	MET	-	EXPRESSION TAG	UNP Q07820
A	173	ASP	-	EXPRESSION TAG	UNP Q07820
B	164	GLY	-	EXPRESSION TAG	UNP Q07820
B	165	THR	-	EXPRESSION TAG	UNP Q07820
B	166	LEU	-	EXPRESSION TAG	UNP Q07820
B	167	VAL	-	EXPRESSION TAG	UNP Q07820
B	168	PRO	-	EXPRESSION TAG	UNP Q07820
B	169	ARG	-	EXPRESSION TAG	UNP Q07820
B	170	GLY	-	EXPRESSION TAG	UNP Q07820

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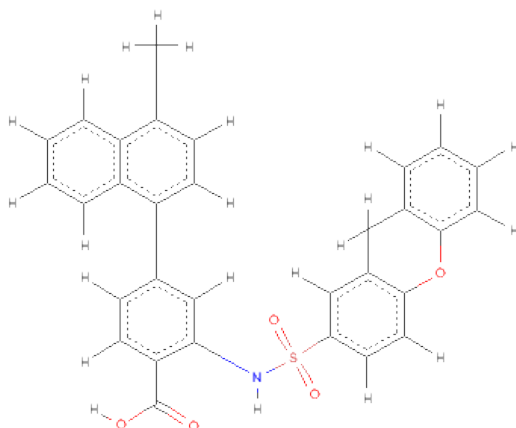
Chain	Residue	Modelled	Actual	Comment	Reference
B	171	SER	-	EXPRESSION TAG	UNP Q07820
B	172	MET	-	EXPRESSION TAG	UNP Q07820
B	173	ASP	-	EXPRESSION TAG	UNP Q07820
C	164	GLY	-	EXPRESSION TAG	UNP Q07820
C	165	THR	-	EXPRESSION TAG	UNP Q07820
C	166	LEU	-	EXPRESSION TAG	UNP Q07820
C	167	VAL	-	EXPRESSION TAG	UNP Q07820
C	168	PRO	-	EXPRESSION TAG	UNP Q07820
C	169	ARG	-	EXPRESSION TAG	UNP Q07820
C	170	GLY	-	EXPRESSION TAG	UNP Q07820
C	171	SER	-	EXPRESSION TAG	UNP Q07820
C	172	MET	-	EXPRESSION TAG	UNP Q07820
C	173	ASP	-	EXPRESSION TAG	UNP Q07820
D	164	GLY	-	EXPRESSION TAG	UNP Q07820
D	165	THR	-	EXPRESSION TAG	UNP Q07820
D	166	LEU	-	EXPRESSION TAG	UNP Q07820
D	167	VAL	-	EXPRESSION TAG	UNP Q07820
D	168	PRO	-	EXPRESSION TAG	UNP Q07820
D	169	ARG	-	EXPRESSION TAG	UNP Q07820
D	170	GLY	-	EXPRESSION TAG	UNP Q07820
D	171	SER	-	EXPRESSION TAG	UNP Q07820
D	172	MET	-	EXPRESSION TAG	UNP Q07820
D	173	ASP	-	EXPRESSION TAG	UNP Q07820
E	164	GLY	-	EXPRESSION TAG	UNP Q07820
E	165	THR	-	EXPRESSION TAG	UNP Q07820
E	166	LEU	-	EXPRESSION TAG	UNP Q07820
E	167	VAL	-	EXPRESSION TAG	UNP Q07820
E	168	PRO	-	EXPRESSION TAG	UNP Q07820
E	169	ARG	-	EXPRESSION TAG	UNP Q07820
E	170	GLY	-	EXPRESSION TAG	UNP Q07820
E	171	SER	-	EXPRESSION TAG	UNP Q07820
E	172	MET	-	EXPRESSION TAG	UNP Q07820
E	173	ASP	-	EXPRESSION TAG	UNP Q07820
F	164	GLY	-	EXPRESSION TAG	UNP Q07820
F	165	THR	-	EXPRESSION TAG	UNP Q07820
F	166	LEU	-	EXPRESSION TAG	UNP Q07820
F	167	VAL	-	EXPRESSION TAG	UNP Q07820
F	168	PRO	-	EXPRESSION TAG	UNP Q07820
F	169	ARG	-	EXPRESSION TAG	UNP Q07820
F	170	GLY	-	EXPRESSION TAG	UNP Q07820
F	171	SER	-	EXPRESSION TAG	UNP Q07820
F	172	MET	-	EXPRESSION TAG	UNP Q07820

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Chain	Residue	Modelled	Actual	Comment	Reference
F	173	ASP	-	EXPRESSION TAG	UNP Q07820

- Molecule 2 is 4-(4-METHYLNAPHTHALEN-1-YL)-2-{[(4-PHENOXYPHENYL)SULFONYL]AMINO}BENZOICACID (three-letter code: 2UU) (formula: C<sub>30</sub>H<sub>23</sub>NO<sub>5</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		
2	B	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		
2	C	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		
2	D	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		
2	E	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		
2	F	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O	0	0
			27 27		
3	B	27	Total O	0	0
			27 27		

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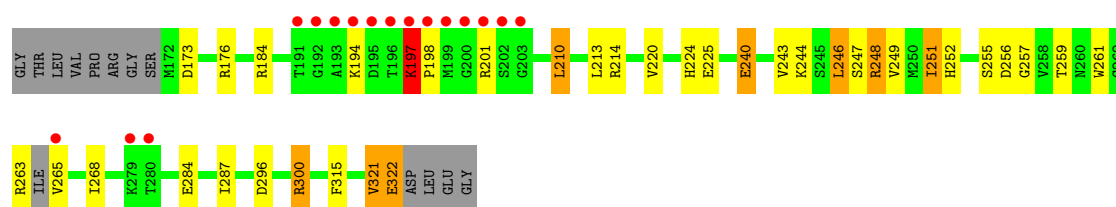
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	23	Total 23	O 23	0	0
3	D	26	Total 26	O 26	0	0
3	E	30	Total 30	O 30	0	0
3	F	21	Total 21	O 21	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

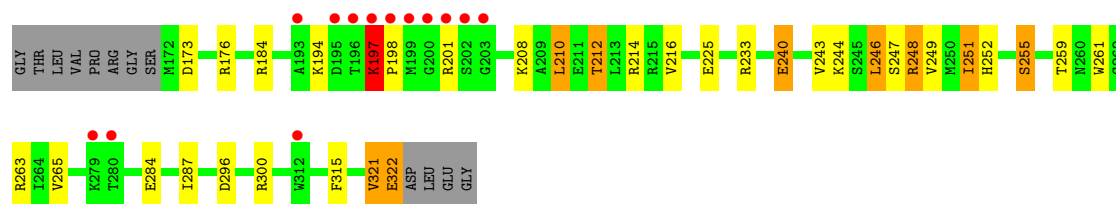
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A: 



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain B: 



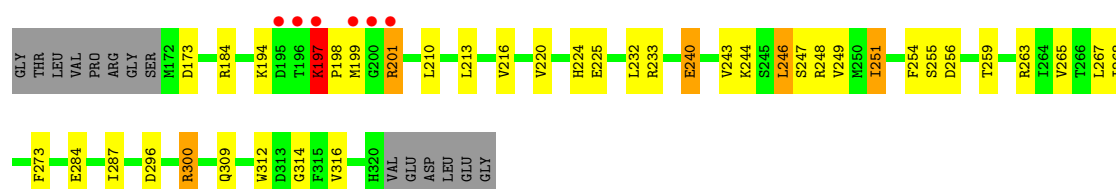
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain C: 



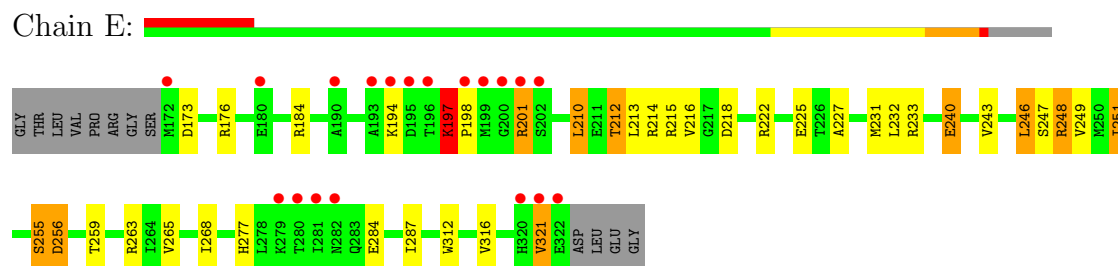
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain D: 



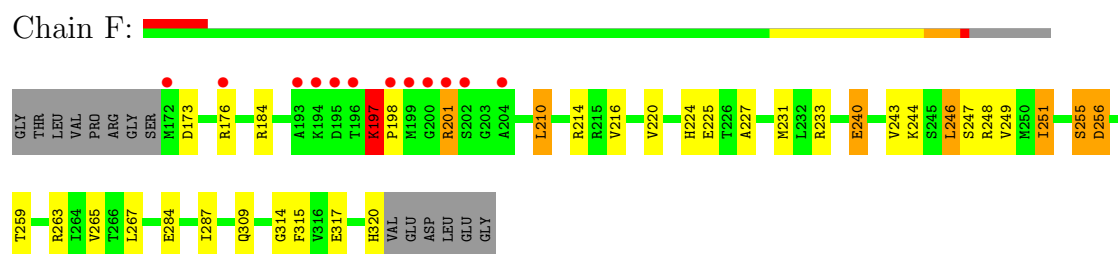
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain E:



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.11Å 109.75Å 76.54Å 90.00° 93.31° 90.00°	Depositor
Resolution (Å)	48.15 – 2.86 48.15 – 2.86	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.15-2.86) 97.8 (48.15-2.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, $R_{free}$	0.198 , 0.239 0.195 , 0.235	Depositor DCC
$R_{free}$ test set	1341 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 26747 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	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 52.67 % 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 4.7063e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2UU

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	0.52	0/1227	0.71	0/1647
1	B	0.52	0/1236	0.70	0/1661
1	C	0.52	0/1220	0.71	0/1639
1	D	0.53	0/1220	0.71	0/1639
1	E	0.51	0/1236	0.69	0/1661
1	F	0.50	0/1220	0.69	0/1639
All	All	0.52	0/7359	0.70	0/9886

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1208	0	1217	30	0
1	B	1216	0	1229	27	0
1	C	1200	0	1214	21	0
1	D	1200	0	1214	24	0
1	E	1216	0	1229	24	0
1	F	1200	0	1214	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	37	20	0	1	0
2	B	37	20	0	1	0
2	C	37	20	0	1	0
2	D	37	20	0	3	0
2	E	37	20	0	1	0
2	F	37	20	0	1	0
3	A	27	0	0	1	0
3	B	27	0	0	0	0
3	C	23	0	0	1	0
3	D	26	0	0	1	0
3	E	30	0	0	1	0
3	F	21	0	0	0	0
All	All	7616	120	7317	135	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (135) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:184:ARG:HH21	1:A:198:PRO:HD2	1.50	0.76
1:B:184:ARG:HH21	1:B:198:PRO:HD2	1.51	0.75
1:A:197:LYS:HB2	1:A:198:PRO:HD3	1.69	0.74
1:B:197:LYS:HB2	1:B:198:PRO:HD3	1.70	0.74
1:E:184:ARG:HH21	1:E:198:PRO:HD2	1.52	0.73
1:E:197:LYS:HB2	1:E:198:PRO:HD3	1.69	0.73
1:D:184:ARG:HH21	1:D:198:PRO:HD2	1.53	0.72
1:F:184:ARG:HH21	1:F:198:PRO:HD2	1.53	0.72
1:F:197:LYS:HB2	1:F:198:PRO:HD3	1.71	0.71
1:C:197:LYS:HB2	1:C:198:PRO:HD3	1.70	0.71
1:D:197:LYS:HB2	1:D:198:PRO:HD3	1.71	0.71
1:C:184:ARG:HH21	1:C:198:PRO:HD2	1.52	0.71
1:D:199:MET:HA	3:D:524:HOH:O	1.92	0.69
1:A:300:ARG:HD3	1:B:255:SER:CB	2.23	0.68
1:A:300:ARG:HD3	1:B:255:SER:HB3	1.77	0.66
1:B:321:VAL:HG23	1:B:322:GLU:H	1.59	0.66
1:E:243:VAL:HA	1:E:246:LEU:HD22	1.80	0.64
1:B:216:VAL:HG12	1:B:265:VAL:HG11	1.79	0.63
1:A:256:ASP:HA	1:B:300:ARG:NH2	2.15	0.61
1:A:261:TRP:O	1:A:265:VAL:HG23	2.03	0.59
1:B:208:LYS:O	1:B:212:THR:HG23	2.01	0.59
1:F:216:VAL:HG12	1:F:265:VAL:HG11	1.84	0.59
1:E:227:ALA:O	1:E:231:MET:HG3	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:220:VAL:O	1:C:224:HIS:HD2	1.87	0.58
1:D:243:VAL:HA	1:D:246:LEU:HD22	1.85	0.58
1:C:212:THR:HG22	1:C:215:ARG:NH2	2.19	0.58
1:E:247:SER:O	1:E:251:ILE:HG13	2.05	0.57
1:E:232:LEU:HD21	1:E:277:HIS:HB2	1.87	0.57
1:C:243:VAL:HA	1:C:246:LEU:HD22	1.86	0.56
1:D:216:VAL:HG12	1:D:265:VAL:HG11	1.86	0.56
1:D:220:VAL:O	1:D:224:HIS:HD2	1.89	0.56
1:D:247:SER:O	1:D:251:ILE:HG13	2.05	0.56
1:F:243:VAL:HA	1:F:246:LEU:HD22	1.88	0.55
1:A:247:SER:O	1:A:251:ILE:HG13	2.06	0.55
1:C:216:VAL:HG12	1:C:265:VAL:HG11	1.88	0.55
1:C:247:SER:O	1:C:251:ILE:HG13	2.06	0.55
1:E:212:THR:HG22	1:E:215:ARG:NH2	2.22	0.55
1:D:246:LEU:HG	2:D:401:2UU:H7	1.89	0.54
1:A:243:VAL:HA	1:A:246:LEU:HD22	1.88	0.54
1:C:184:ARG:NH2	1:C:198:PRO:HD2	2.23	0.54
1:B:243:VAL:HA	1:B:246:LEU:HD22	1.89	0.54
1:B:247:SER:O	1:B:251:ILE:HG13	2.08	0.54
1:B:261:TRP:CZ3	1:B:315:PHE:HB2	2.43	0.54
1:D:296:ASP:O	1:D:300:ARG:HB2	2.07	0.54
1:B:184:ARG:NH2	1:B:198:PRO:HD2	2.21	0.53
1:A:213:LEU:HD21	1:A:268:ILE:HG21	1.90	0.53
1:E:184:ARG:NH2	1:E:198:PRO:HD2	2.23	0.53
1:F:255:SER:O	1:F:256:ASP:C	2.46	0.53
1:F:184:ARG:NH2	1:F:198:PRO:HD2	2.23	0.53
1:F:247:SER:O	1:F:251:ILE:HG13	2.09	0.53
1:E:216:VAL:HG12	1:E:265:VAL:HG11	1.90	0.52
1:D:213:LEU:HD21	1:D:268:ILE:HG21	1.92	0.52
1:D:300:ARG:HG2	1:E:255:SER:CB	2.40	0.52
1:C:213:LEU:HD21	1:C:268:ILE:HG21	1.92	0.51
1:B:210:LEU:O	1:B:214:ARG:HG2	2.11	0.50
1:A:321:VAL:HG23	1:A:322:GLU:H	1.76	0.50
1:A:246:LEU:HG	2:A:401:2UU:H7	1.93	0.50
1:F:255:SER:O	1:F:256:ASP:O	2.30	0.50
1:F:227:ALA:O	1:F:231:MET:HG3	2.12	0.49
1:A:296:ASP:OD2	1:B:252:HIS:HD2	1.95	0.49
1:E:255:SER:O	1:E:256:ASP:C	2.50	0.49
1:C:248:ARG:HD2	1:F:244:LYS:HG2	1.95	0.49
1:B:243:VAL:O	1:B:246:LEU:HB2	2.13	0.48
1:E:255:SER:O	1:E:256:ASP:O	2.31	0.48
1:C:309:GLN:O	1:C:314:GLY:HA3	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:184:ARG:NH2	1:A:198:PRO:HD2	2.23	0.48
1:D:312:TRP:O	1:D:316:VAL:HG23	2.14	0.48
1:A:214:ARG:HD2	3:A:523:HOH:O	2.12	0.48
1:C:210:LEU:HD13	1:C:214:ARG:NH2	2.28	0.47
1:D:184:ARG:NH2	1:D:198:PRO:HD2	2.23	0.47
1:A:261:TRP:O	1:A:265:VAL:CG2	2.62	0.47
1:D:197:LYS:CB	1:D:198:PRO:HD3	2.43	0.47
1:A:210:LEU:CD1	1:A:214:ARG:NH2	2.78	0.47
1:A:197:LYS:CB	1:A:198:PRO:HD3	2.42	0.47
1:A:248:ARG:HD2	1:B:244:LYS:HG2	1.95	0.47
1:F:197:LYS:CB	1:F:198:PRO:HD3	2.44	0.47
1:C:243:VAL:O	1:C:246:LEU:HB2	2.14	0.47
1:A:252:HIS:HD2	1:B:296:ASP:OD2	1.98	0.46
1:A:257:GLY:HA3	1:F:233:ARG:NH2	2.30	0.46
1:D:309:GLN:O	1:D:314:GLY:HA3	2.15	0.46
1:C:255:SER:O	1:C:256:ASP:HB3	2.16	0.46
1:B:197:LYS:CB	1:B:198:PRO:HD3	2.43	0.46
1:D:220:VAL:O	1:D:224:HIS:CD2	2.68	0.46
1:C:249:VAL:HG22	3:C:520:HOH:O	2.15	0.46
1:C:220:VAL:O	1:C:224:HIS:CD2	2.67	0.46
1:A:251:ILE:HD11	1:B:251:ILE:HD11	1.98	0.45
1:B:265:VAL:HG22	1:B:315:PHE:HE1	1.81	0.45
1:D:254:PHE:HA	2:D:401:2UU:O32	2.17	0.45
1:F:243:VAL:O	1:F:246:LEU:HB2	2.17	0.45
1:E:197:LYS:CB	1:E:198:PRO:HD3	2.42	0.45
1:A:265:VAL:HG22	1:A:315:PHE:HE1	1.82	0.45
1:E:210:LEU:HD12	1:E:214:ARG:NH2	2.32	0.45
1:F:210:LEU:O	1:F:214:ARG:HG2	2.17	0.44
1:E:210:LEU:O	1:E:214:ARG:HG2	2.17	0.44
1:A:284:GLU:HA	1:A:287:ILE:HD12	2.00	0.44
1:C:246:LEU:HG	2:C:401:2UU:H7	1.98	0.43
1:E:312:TRP:O	1:E:316:VAL:HG23	2.18	0.43
1:A:243:VAL:O	1:A:246:LEU:HB2	2.18	0.43
1:C:197:LYS:CB	1:C:198:PRO:HD3	2.43	0.43
1:A:220:VAL:O	1:A:224:HIS:HD2	2.00	0.43
1:E:284:GLU:HA	1:E:287:ILE:HD12	2.00	0.43
1:D:240:GLU:CD	1:D:240:GLU:H	2.22	0.43
1:F:246:LEU:HG	2:F:401:2UU:H7	2.00	0.43
1:B:240:GLU:H	1:B:240:GLU:CD	2.22	0.43
1:F:240:GLU:CD	1:F:240:GLU:H	2.23	0.42
1:F:309:GLN:O	1:F:314:GLY:HA3	2.20	0.42
1:F:220:VAL:O	1:F:224:HIS:CD2	2.73	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:220:VAL:O	1:F:224:HIS:HD2	2.02	0.42
1:C:197:LYS:HB2	1:C:198:PRO:CD	2.46	0.42
1:D:267:LEU:HD12	2:D:401:2UU:C8	2.50	0.42
1:B:246:LEU:HG	2:B:401:2UU:H7	2.02	0.42
1:A:244:LYS:HG2	1:B:248:ARG:HD2	2.01	0.42
1:A:240:GLU:CD	1:A:240:GLU:H	2.23	0.42
1:C:240:GLU:H	1:C:240:GLU:CD	2.23	0.42
1:D:244:LYS:HG2	1:E:248:ARG:HD2	2.02	0.42
1:F:284:GLU:HA	1:F:287:ILE:HD12	2.01	0.42
1:E:240:GLU:CD	1:E:240:GLU:H	2.22	0.42
1:E:218:ASP:OD1	1:E:222:ARG:HD2	2.20	0.41
1:E:176:ARG:HH11	1:E:201:ARG:HE	1.69	0.41
1:D:197:LYS:HB2	1:D:198:PRO:CD	2.47	0.41
1:D:243:VAL:O	1:D:246:LEU:HB2	2.19	0.41
1:B:284:GLU:HA	1:B:287:ILE:HD12	2.03	0.41
1:A:300:ARG:HD3	1:B:255:SER:OG	2.20	0.41
1:B:197:LYS:HB2	1:B:198:PRO:CD	2.46	0.41
1:D:232:LEU:HD22	1:D:273:PHE:CE2	2.56	0.41
1:E:213:LEU:HD21	1:E:268:ILE:HG21	2.02	0.41
1:F:176:ARG:HH11	1:F:201:ARG:HE	1.69	0.41
1:C:284:GLU:HA	1:C:287:ILE:HD12	2.03	0.40
1:F:265:VAL:CG2	1:F:315:PHE:HE1	2.35	0.40
1:E:246:LEU:HG	2:E:401:2UU:H7	2.02	0.40
1:E:247:SER:HB2	3:E:507:HOH:O	2.20	0.40
1:D:284:GLU:HA	1:D:287:ILE:HD12	2.02	0.40
1:A:261:TRP:CZ3	1:A:315:PHE:HB2	2.56	0.40
1:A:176:ARG:HH11	1:A:201:ARG:HE	1.69	0.40
1:B:176:ARG:HH11	1:B:201:ARG:HE	1.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	146/163 (90%)	136 (93%)	7 (5%)	3 (2%)	11 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	149/163 (91%)	139 (93%)	7 (5%)	3 (2%)	11	37
1	C	147/163 (90%)	140 (95%)	5 (3%)	2 (1%)	16	49
1	D	147/163 (90%)	139 (95%)	4 (3%)	4 (3%)	8	28
1	E	149/163 (91%)	138 (93%)	7 (5%)	4 (3%)	8	28
1	F	147/163 (90%)	138 (94%)	6 (4%)	3 (2%)	11	37
All	All	885/978 (90%)	830 (94%)	36 (4%)	19 (2%)	11	36

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	LYS
1	B	197	LYS
1	C	197	LYS
1	D	197	LYS
1	E	197	LYS
1	E	256	ASP
1	F	197	LYS
1	F	256	ASP
1	C	200	GLY
1	E	321	VAL
1	D	201	ARG
1	A	255	SER
1	B	255	SER
1	D	255	SER
1	E	255	SER
1	F	255	SER
1	D	256	ASP
1	A	321	VAL
1	B	321	VAL

### 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	131/141 (93%)	117 (89%)	14 (11%)	10	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	132/141 (94%)	117 (89%)	15 (11%)	8	22
1	C	130/141 (92%)	116 (89%)	14 (11%)	9	25
1	D	130/141 (92%)	115 (88%)	15 (12%)	8	22
1	E	132/141 (94%)	116 (88%)	16 (12%)	7	19
1	F	130/141 (92%)	115 (88%)	15 (12%)	8	22
All	All	785/846 (93%)	696 (89%)	89 (11%)	9	23

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ASP
1	A	194	LYS
1	A	197	LYS
1	A	210	LEU
1	A	225	GLU
1	A	240	GLU
1	A	246	LEU
1	A	248	ARG
1	A	249	VAL
1	A	251	ILE
1	A	259	THR
1	A	263	ARG
1	A	300	ARG
1	A	322	GLU
1	B	173	ASP
1	B	194	LYS
1	B	197	LYS
1	B	210	LEU
1	B	212	THR
1	B	225	GLU
1	B	233	ARG
1	B	240	GLU
1	B	246	LEU
1	B	248	ARG
1	B	249	VAL
1	B	251	ILE
1	B	259	THR
1	B	263	ARG
1	B	322	GLU
1	C	173	ASP

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Mol	Chain	Res	Type
1	C	194	LYS
1	C	197	LYS
1	C	210	LEU
1	C	212	THR
1	C	225	GLU
1	C	233	ARG
1	C	240	GLU
1	C	246	LEU
1	C	248	ARG
1	C	249	VAL
1	C	251	ILE
1	C	259	THR
1	C	263	ARG
1	D	173	ASP
1	D	194	LYS
1	D	197	LYS
1	D	201	ARG
1	D	210	LEU
1	D	225	GLU
1	D	233	ARG
1	D	240	GLU
1	D	246	LEU
1	D	248	ARG
1	D	249	VAL
1	D	251	ILE
1	D	259	THR
1	D	263	ARG
1	D	300	ARG
1	E	173	ASP
1	E	194	LYS
1	E	197	LYS
1	E	201	ARG
1	E	210	LEU
1	E	212	THR
1	E	225	GLU
1	E	233	ARG
1	E	240	GLU
1	E	246	LEU
1	E	248	ARG
1	E	249	VAL
1	E	251	ILE
1	E	259	THR

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Mol	Chain	Res	Type
1	E	263	ARG
1	E	321	VAL
1	F	173	ASP
1	F	197	LYS
1	F	201	ARG
1	F	210	LEU
1	F	225	GLU
1	F	240	GLU
1	F	246	LEU
1	F	248	ARG
1	F	249	VAL
1	F	251	ILE
1	F	259	THR
1	F	263	ARG
1	F	267	LEU
1	F	317	GLU
1	F	320	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	HIS
1	A	239	ASN
1	A	252	HIS
1	B	177	GLN
1	B	239	ASN
1	B	252	HIS
1	C	177	GLN
1	C	224	HIS
1	C	239	ASN
1	D	224	HIS
1	D	239	ASN
1	D	252	HIS
1	E	177	GLN
1	E	224	HIS
1	E	239	ASN
1	E	252	HIS
1	F	224	HIS
1	F	239	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands 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$
2	2UU	A	401	-	41,41,41	1.35	4 (9%)	59,59,59	0.99	2 (3%)
2	2UU	B	401	-	41,41,41	1.15	3 (7%)	59,59,59	0.99	2 (3%)
2	2UU	C	401	-	41,41,41	1.36	3 (7%)	59,59,59	0.88	1 (1%)
2	2UU	D	401	-	41,41,41	1.30	2 (4%)	59,59,59	1.01	1 (1%)
2	2UU	E	401	-	41,41,41	1.34	3 (7%)	59,59,59	0.88	2 (3%)
2	2UU	F	401	-	41,41,41	1.33	4 (9%)	59,59,59	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
2	2UU	A	401	-	-	0/23/23/23	0/5/5/5
2	2UU	B	401	-	-	0/23/23/23	0/5/5/5
2	2UU	C	401	-	-	0/23/23/23	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2UU	D	401	-	-	0/23/23/23	0/5/5/5
2	2UU	E	401	-	-	0/23/23/23	0/5/5/5
2	2UU	F	401	-	-	0/23/23/23	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	2UU	S37-N31	5.51	1.72	1.63
2	E	401	2UU	S37-N31	5.42	1.72	1.63
2	A	401	2UU	S37-N31	5.23	1.72	1.63
2	D	401	2UU	S37-N31	4.74	1.71	1.63
2	F	401	2UU	S37-N31	4.61	1.71	1.63
2	B	401	2UU	S37-N31	4.08	1.70	1.63
2	F	401	2UU	C22-C21	-3.60	1.43	1.49
2	D	401	2UU	C22-C21	-3.59	1.43	1.49
2	E	401	2UU	C22-C21	-3.56	1.43	1.49
2	C	401	2UU	C22-C21	-3.26	1.43	1.49
2	A	401	2UU	C22-C21	-2.70	1.44	1.49
2	B	401	2UU	C22-C21	-2.66	1.44	1.49
2	A	401	2UU	C20-C19	-2.47	1.38	1.43
2	F	401	2UU	C24-C20	-2.27	1.38	1.42
2	C	401	2UU	C20-C19	-2.14	1.39	1.43
2	A	401	2UU	C24-C20	-2.13	1.38	1.42
2	F	401	2UU	C7-C20	-2.03	1.38	1.42
2	E	401	2UU	C20-C19	-2.01	1.39	1.43
2	B	401	2UU	O33-S37	2.01	1.45	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	2UU	C25-C23-C29	3.04	126.53	121.86
2	A	401	2UU	O33-S37-O34	2.62	123.00	119.55
2	C	401	2UU	O35-C29-C23	-2.52	108.05	115.48
2	B	401	2UU	C18-C21-C22	-2.18	117.16	120.63
2	A	401	2UU	C25-N31-S37	-2.16	116.76	123.57
2	E	401	2UU	C30-C24-C20	2.13	124.31	120.97
2	E	401	2UU	O35-C29-C23	-2.01	109.55	115.48
2	B	401	2UU	C28-S37-N31	-2.01	104.48	106.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	150/163 (92%)	0.56	16 (10%) 6 8	36, 53, 110, 141	0
1	B	151/163 (92%)	0.46	13 (8%) 11 12	35, 51, 110, 137	0
1	C	149/163 (91%)	0.15	7 (4%) 30 37	37, 56, 101, 126	0
1	D	149/163 (91%)	0.14	6 (4%) 36 43	37, 52, 101, 132	0
1	E	151/163 (92%)	0.52	19 (12%) 4 5	38, 59, 110, 134	0
1	F	149/163 (91%)	0.50	12 (8%) 12 14	39, 60, 114, 136	0
All	All	899/978 (91%)	0.39	73 (8%) 12 14	35, 55, 110, 141	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	201	ARG	9.8
1	C	201	ARG	9.3
1	A	201	ARG	8.2
1	F	201	ARG	7.9
1	B	200	GLY	7.8
1	D	200	GLY	7.4
1	B	201	ARG	7.3
1	D	201	ARG	7.0
1	B	198	PRO	6.3
1	F	200	GLY	6.2
1	E	202	SER	5.7
1	F	193	ALA	5.4
1	A	200	GLY	5.4
1	F	198	PRO	5.3
1	A	198	PRO	5.1
1	B	196	THR	4.8
1	C	200	GLY	4.8
1	B	202	SER	4.8
1	E	200	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	203	GLY	4.5
1	E	198	PRO	4.3
1	B	199	MET	4.3
1	A	199	MET	4.3
1	E	199	MET	4.1
1	F	199	MET	4.1
1	F	195	ASP	4.0
1	D	199	MET	4.0
1	E	321	VAL	4.0
1	A	202	SER	3.8
1	D	196	THR	3.7
1	A	193	ALA	3.6
1	A	280	THR	3.6
1	F	202	SER	3.6
1	C	195	ASP	3.6
1	E	322	GLU	3.4
1	A	195	ASP	3.4
1	C	196	THR	3.4
1	F	196	THR	3.3
1	D	195	ASP	3.3
1	C	199	MET	3.2
1	C	193	ALA	3.1
1	A	197	LYS	3.1
1	B	280	THR	3.0
1	E	196	THR	2.9
1	B	195	ASP	2.9
1	F	172	MET	2.9
1	E	282	ASN	2.9
1	B	193	ALA	2.8
1	E	194	LYS	2.8
1	B	197	LYS	2.7
1	A	203	GLY	2.7
1	E	193	ALA	2.7
1	E	172	MET	2.6
1	E	320	HIS	2.6
1	F	194	LYS	2.5
1	E	190	ALA	2.4
1	E	195	ASP	2.4
1	A	265	VAL	2.4
1	A	279	LYS	2.4
1	A	196	THR	2.3
1	E	280	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	194	LYS	2.2
1	D	197	LYS	2.2
1	F	204	ALA	2.2
1	B	279	LYS	2.2
1	A	192	GLY	2.2
1	A	191	THR	2.2
1	E	279	LYS	2.1
1	F	176	ARG	2.1
1	E	180	GLU	2.1
1	E	281	ILE	2.0
1	B	312	TRP	2.0
1	C	198	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	2UU	D	401	37/37	0.19	0.45	35,44,64,64	0
2	2UU	C	401	37/37	0.19	0.42	38,45,56,57	0
2	2UU	F	401	37/37	0.17	-0.25	38,44,49,50	0
2	2UU	A	401	37/37	0.17	-0.79	35,42,50,50	0
2	2UU	E	401	37/37	0.15	-1.10	35,46,51,53	0
2	2UU	B	401	37/37	0.15	-1.23	35,40,45,46	0



## 6.5 Other polymers ⓘ

There are no such residues in this entry.