



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 07:56 PM BST

PDB ID : 3V62  
Title : Structure of the *S. cerevisiae* Srs2 C-terminal domain in complex with PCNA conjugated to SUMO on lysine 164  
Authors : Armstrong, A.A.; Mohideen, F.; Lima, C.D.  
Deposited on : 2011-12-18  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

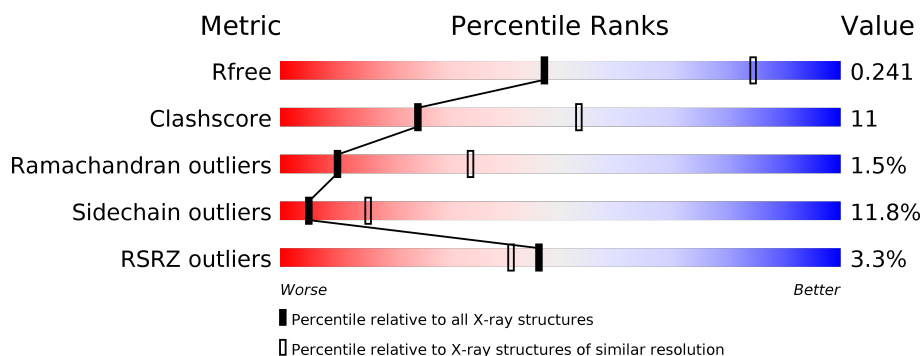
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	84	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>6%</div> </div> </div>
1	D	84	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>30%</div> <div>6%</div> </div> </div>
2	B	258	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>5%</div> </div> </div>
2	E	258	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>5%</div> </div> </div>
3	C	69	<div> <div>6%</div> <div> <div></div> <div>23%</div> <div>6%</div> <div>70%</div> </div> </div>
3	F	69	<div> <div>0%</div> <div> <div></div> <div>22%</div> <div>7%</div> <div>70%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5723 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 Ubiquitin-like protein SMT3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	79	Total	C	N	O	S	0	0	0
			644	404	113	124	3			
1	D	79	Total	C	N	O	S	0	0	0
			644	404	113	124	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	EXPRESSION TAG	UNP Q12306
A	16	SER	-	EXPRESSION TAG	UNP Q12306
A	17	HIS	-	EXPRESSION TAG	UNP Q12306
A	18	MET	-	EXPRESSION TAG	UNP Q12306
A	19	ARG	-	EXPRESSION TAG	UNP Q12306
D	15	GLY	-	EXPRESSION TAG	UNP Q12306
D	16	SER	-	EXPRESSION TAG	UNP Q12306
D	17	HIS	-	EXPRESSION TAG	UNP Q12306
D	18	MET	-	EXPRESSION TAG	UNP Q12306
D	19	ARG	-	EXPRESSION TAG	UNP Q12306

- Molecule 2 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	255	Total	C	N	O	S	0	0	0
			1998	1277	315	396	10			
2	E	255	Total	C	N	O	S	0	0	0
			1998	1277	315	396	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	127	GLY	LYS	ENGINEERED MUTATION	UNP P15873
E	127	GLY	LYS	ENGINEERED MUTATION	UNP P15873

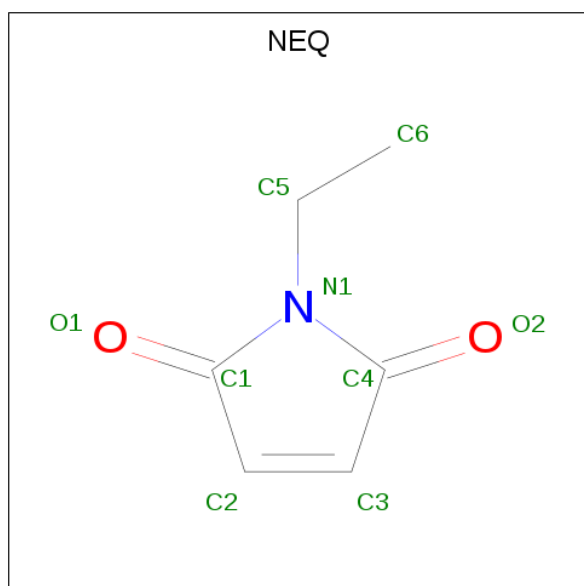
- Molecule 3 is a protein called ATP-dependent DNA helicase SRS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	21	Total	C	N	O	S	0	0	0
			166	104	28	33	1			
3	F	21	Total	C	N	O	S	0	0	0
			166	104	28	33	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1106	SER	-	EXPRESSION TAG	UNP P12954
F	1106	SER	-	EXPRESSION TAG	UNP P12954

- Molecule 4 is N-ETHYLMALEIMIDE (three-letter code: NEQ) (formula:  $C_6H_7NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			9	6	1	2		
4	B	1	Total	C	N	O	0	0
			9	6	1	2		
4	E	1	Total	C	N	O	0	0
			9	6	1	2		
4	E	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

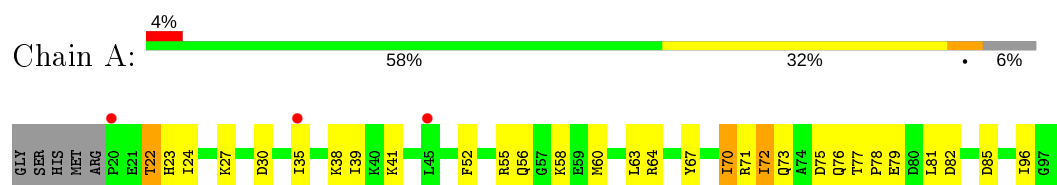
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	24	Total	O	0	0
			24	24		
6	D	1	Total	O	0	0
			1	1		
6	E	18	Total	O	0	0
			18	18		
6	F	2	Total	O	0	0
			2	2		

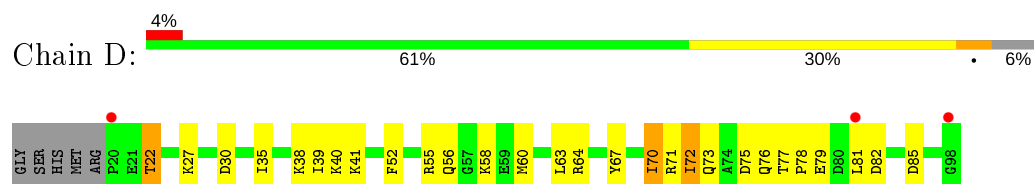
### 3 Residue-property plots [i](#)

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.

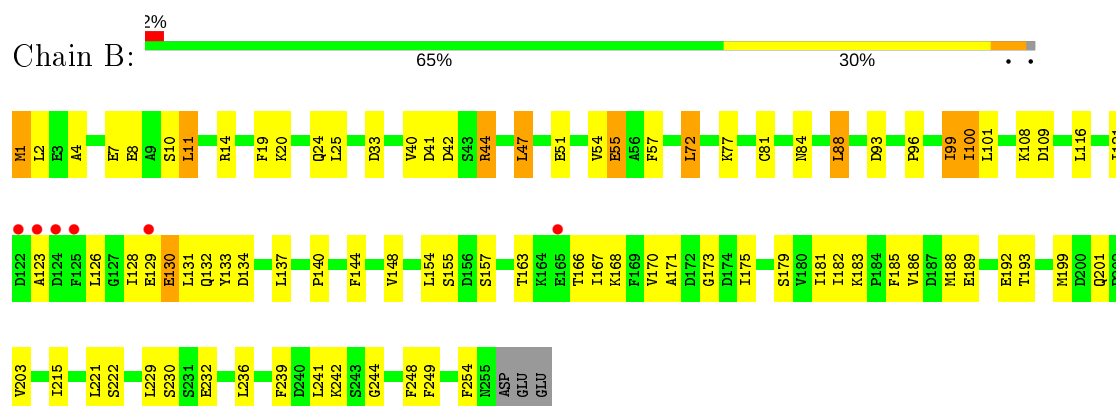
- Molecule 1: Ubiquitin-like protein SMT3



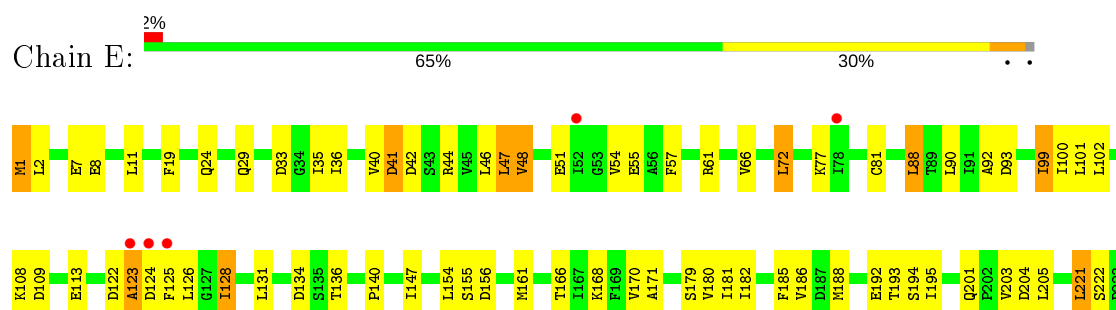
- Molecule 1: Ubiquitin-like protein SMT3

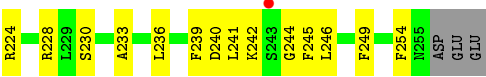


- Molecule 2: Proliferating cell nuclear antigen



- Molecule 2: Proliferating cell nuclear antigen

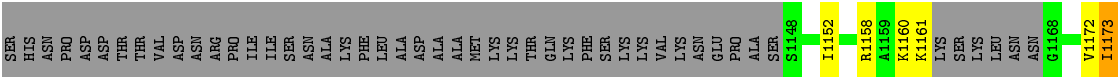




• Molecule 3: ATP-dependent DNA helicase SRS2



• Molecule 3: ATP-dependent DNA helicase SRS2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	196.82Å 62.26Å 139.25Å 90.00° 135.04° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 44.03 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.90) 98.8 (44.03-2.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.184 , 0.237 0.187 , 0.241	Depositor DCC
$R_{free}$ test set	1343 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.467 for h+2*l,k,-h-l 0.019 for -h,-k,h+l 0.023 for h+2*l,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5723	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLY, SO4, NEQ

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	0.44	0/586	0.60	0/788
1	D	0.43	0/586	0.60	0/788
2	B	0.49	0/2028	0.69	1/2736 (0.0%)
2	E	0.49	0/2028	0.69	1/2736 (0.0%)
3	C	0.39	0/165	0.53	0/215
3	F	0.37	0/165	0.52	0/215
All	All	0.47	0/5558	0.66	2/7478 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	126	LEU	CA-CB-CG	5.45	127.83	115.30
2	E	126	LEU	CA-CB-CG	5.16	127.16	115.30

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	644	0	636	19	0
1	D	644	0	636	15	0
2	B	1998	0	2010	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1998	0	2010	44	0
3	C	166	0	172	7	0
3	F	166	0	172	6	0
4	B	18	0	12	0	0
4	E	18	0	12	0	0
5	B	10	0	0	0	0
5	E	10	0	0	0	0
6	A	6	0	0	0	0
6	B	24	0	0	1	0
6	D	1	0	0	0	0
6	E	18	0	0	0	0
6	F	2	0	0	0	0
All	All	5723	0	5660	123	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (123) 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)
2:E:134:ASP:HB3	2:E:201:GLN:HB3	1.61	0.81
2:B:168:LYS:HG3	2:B:181:ILE:HG12	1.67	0.76
2:E:40:VAL:HG12	2:E:123:ALA:HB2	1.68	0.76
1:A:38:MLY:HB2	3:C:1172:VAL:HG13	1.71	0.72
1:D:38:MLY:HB2	3:F:1172:VAL:HG13	1.70	0.72
2:E:222:SER:HB3	2:E:239:PHE:HB3	1.71	0.72
1:D:67:TYR:HB2	1:D:72:ILE:HD11	1.72	0.71
1:A:67:TYR:HB2	1:A:72:ILE:HD11	1.74	0.69
2:B:163:THR:OG1	2:B:166:THR:HB	1.94	0.68
2:B:170:VAL:HG22	2:B:179:SER:HB3	1.75	0.68
2:E:24:GLN:O	2:E:72:LEU:HB2	1.94	0.67
1:D:73:GLN:O	1:D:76:GLN:HG2	1.94	0.67
2:E:170:VAL:HG22	2:E:179:SER:HB3	1.77	0.67
2:E:236:LEU:HD13	2:E:249:PHE:CE2	2.31	0.66
1:A:73:GLN:O	1:A:76:GLN:HG2	1.96	0.66
2:B:40:VAL:HG12	2:B:123:ALA:HB2	1.79	0.64
1:A:70:ILE:HG21	2:B:186:VAL:HG23	1.79	0.64
2:B:134:ASP:HB3	2:B:201:GLN:HB3	1.79	0.64
2:E:1:MET:HB2	2:E:93:ASP:HA	1.81	0.62
1:A:30:ASP:OD2	1:A:58:MLY:HH21	2.01	0.60
1:D:30:ASP:OD2	1:D:58:MLY:HH21	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:LEU:HD13	2:B:249:PHE:CE2	2.35	0.60
2:B:221:LEU:HB3	2:B:241:LEU:HD22	1.83	0.59
1:D:70:ILE:HG21	2:E:186:VAL:HG23	1.85	0.59
2:E:99:ILE:HG12	2:E:100:ILE:N	2.18	0.59
2:B:51:GLU:O	2:B:244:GLY:HA3	2.04	0.58
2:B:10:SER:HB3	2:B:84:ASN:HB3	1.86	0.57
2:E:108:LYS:O	2:E:109:ASP:HB2	2.04	0.57
2:E:222:SER:CB	2:E:239:PHE:HB3	2.34	0.57
2:B:1:MET:HB2	2:B:93:ASP:HA	1.85	0.56
2:E:168:LYS:HG3	2:E:181:ILE:HG12	1.88	0.56
2:B:140:PRO:HG3	2:B:193:THR:HA	1.89	0.55
2:E:47:LEU:HD13	3:F:1152:ILE:HG12	1.90	0.53
1:A:52:PHE:O	1:A:56:GLN:HG2	2.09	0.53
2:E:102:LEU:HD12	2:E:113:GLU:HB3	1.90	0.53
2:E:240:ASP:OD1	2:E:245:PHE:CZ	2.61	0.53
2:B:221:LEU:HB3	2:B:241:LEU:CD2	2.37	0.53
1:D:39:ILE:HG22	3:F:1173:ILE:HB	1.89	0.53
1:D:35:ILE:HD11	1:D:55:ARG:HG2	1.90	0.53
2:B:99:ILE:HG12	2:B:100:ILE:N	2.23	0.53
2:B:8:GLU:HB2	2:B:11:LEU:HD22	1.91	0.53
2:E:51:GLU:O	2:E:244:GLY:HA3	2.08	0.52
2:B:222:SER:HB3	2:B:239:PHE:HB3	1.92	0.52
1:A:35:ILE:HD11	1:A:55:ARG:HG2	1.92	0.52
2:E:99:ILE:HG12	2:E:100:ILE:H	1.75	0.52
2:B:19:PHE:HB3	2:B:72:LEU:HD21	1.92	0.52
1:D:52:PHE:O	1:D:56:GLN:HG2	2.09	0.51
2:B:55:GLU:H	2:B:55:GLU:CD	2.13	0.51
2:B:24:GLN:O	2:B:72:LEU:HB2	2.11	0.51
1:D:41:MLY:O	1:D:79:GLU:HB2	2.10	0.51
1:A:41:MLY:O	1:A:79:GLU:HB2	2.11	0.50
2:B:222:SER:CB	2:B:239:PHE:HB3	2.42	0.50
2:E:36:ILE:HG12	2:E:51:GLU:HG2	1.93	0.49
2:B:47:LEU:HD13	3:C:1152:ILE:HG12	1.94	0.49
1:D:64:ARG:NH1	1:D:71:ARG:HH11	2.09	0.49
2:B:101:LEU:HD12	2:B:101:LEU:N	2.26	0.49
2:E:140:PRO:HG3	2:E:193:THR:HA	1.94	0.49
2:E:7:GLU:HG2	2:E:8:GLU:HG2	1.95	0.49
1:A:39:ILE:HA	3:C:1173:ILE:O	2.13	0.48
2:B:167:ILE:HB	2:B:182:ILE:HG13	1.96	0.48
2:B:183:LYS:HD3	2:E:109:ASP:HB3	1.95	0.48
2:B:129:GLU:C	2:B:131:LEU:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:GLN:NE2	2:E:124:ASP:OD2	2.47	0.48
1:A:77:THR:HB	1:A:78:PRO:HD2	1.95	0.48
1:D:77:THR:HB	1:D:78:PRO:HD2	1.95	0.48
2:B:232:GLU:N	6:B:409:HOH:O	2.47	0.47
2:E:122:ASP:C	2:E:124:ASP:H	2.17	0.47
1:A:64:ARG:NH1	1:A:71:ARG:HH11	2.11	0.47
2:B:155:SER:HB3	2:B:171:ALA:HB1	1.96	0.47
2:B:7:GLU:HG2	2:B:8:GLU:HG2	1.97	0.47
2:E:122:ASP:O	2:E:125:PHE:HD1	1.98	0.47
2:B:144:PHE:O	2:B:148:VAL:HG23	2.15	0.47
2:E:35:ILE:HD12	2:E:57:PHE:HZ	1.80	0.47
2:B:108:LYS:O	2:B:109:ASP:HB2	2.15	0.46
2:B:128:ILE:HA	3:C:1160:LYS:NZ	2.30	0.46
1:D:64:ARG:HH11	1:D:71:ARG:HH11	1.62	0.46
1:A:64:ARG:HH11	1:A:71:ARG:HH11	1.64	0.46
2:E:19:PHE:HB3	2:E:72:LEU:HD21	1.98	0.46
2:B:4:ALA:HB1	2:B:57:PHE:CE1	2.51	0.46
2:B:44:ARG:O	3:C:1152:ILE:HG22	2.15	0.46
1:A:35:ILE:HD11	1:A:55:ARG:CG	2.47	0.45
1:D:35:ILE:HD11	1:D:55:ARG:CG	2.47	0.45
2:B:132:GLN:HG2	2:B:133:TYR:H	1.83	0.44
3:C:1152:ILE:HG13	3:C:1152:ILE:O	2.17	0.44
2:E:128:ILE:HA	3:F:1160:LYS:NZ	2.32	0.44
2:B:93:ASP:O	2:B:96:PRO:HG3	2.17	0.44
2:E:221:LEU:HB3	2:E:241:LEU:CD2	2.47	0.44
2:E:88:LEU:HD21	2:E:101:LEU:HB3	1.99	0.44
2:B:99:ILE:CG2	2:B:116:LEU:HB3	2.48	0.44
2:B:99:ILE:HG12	2:B:100:ILE:H	1.81	0.43
1:D:81:LEU:O	1:D:82:ASP:HB2	2.18	0.43
2:B:11:LEU:HD12	2:B:14:ARG:HH11	1.84	0.43
2:B:88:LEU:HD21	2:B:101:LEU:HB3	1.99	0.43
2:E:136:THR:HG23	2:E:228:ARG:HG2	2.00	0.43
3:F:1152:ILE:O	3:F:1152:ILE:HG13	2.17	0.43
2:E:161:MET:HG3	2:E:204:ASP:HB2	2.00	0.43
2:E:194:SER:O	2:E:224:ARG:NH2	2.45	0.43
2:B:173:GLY:C	2:B:175:ILE:H	2.21	0.43
2:E:101:LEU:N	2:E:101:LEU:HD12	2.34	0.43
2:E:48:VAL:HG23	2:E:246:LEU:HD11	2.01	0.42
2:E:230:SER:OG	2:E:233:ALA:HB3	2.19	0.42
1:A:23:HIS:HB3	1:A:24:ILE:H	1.60	0.41
1:D:40:MLY:HH23	1:D:40:MLY:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:HG22	3:C:1173:ILE:HB	2.03	0.41
1:A:70:ILE:HD12	1:A:71:ARG:N	2.35	0.41
3:F:1158:ARG:HA	3:F:1161:LYS:HE2	2.01	0.41
1:A:81:LEU:O	1:A:82:ASP:HB2	2.21	0.41
2:E:1:MET:HG3	2:E:92:ALA:O	2.21	0.41
2:E:221:LEU:HB3	2:E:241:LEU:HD22	2.02	0.41
2:E:222:SER:HB2	2:E:240:ASP:O	2.20	0.41
2:E:33:ASP:N	2:E:33:ASP:OD1	2.53	0.41
1:A:96:ILE:O	1:A:96:ILE:HG22	2.20	0.41
2:E:41:ASP:HB3	2:E:46:LEU:HB3	2.03	0.41
1:A:23:HIS:CD2	1:A:38:MLY:HE3	2.57	0.40
2:B:25:LEU:HB3	2:B:121:ILE:CD1	2.52	0.40
2:E:155:SER:HB3	2:E:171:ALA:HB1	2.03	0.40
2:E:90:LEU:HB3	2:E:99:ILE:HD11	2.03	0.40
2:B:128:ILE:C	2:B:130:GLU:H	2.23	0.40
2:B:47:LEU:O	2:B:248:PHE:HA	2.21	0.40
2:B:170:VAL:HG22	2:B:179:SER:CB	2.47	0.40
2:E:147:ILE:HG23	2:E:180:VAL:HG21	2.03	0.40
2:B:33:ASP:N	2:B:33:ASP:OD1	2.53	0.40
2:E:1:MET:CB	2:E:93:ASP:HA	2.50	0.40

There are no symmetry-related clashes.

## 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	71/84 (84%)	57 (80%)	12 (17%)	2 (3%)	5	19
1	D	71/84 (84%)	58 (82%)	11 (16%)	2 (3%)	5	19
2	B	253/258 (98%)	228 (90%)	22 (9%)	3 (1%)	13	40
2	E	253/258 (98%)	228 (90%)	22 (9%)	3 (1%)	13	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	17/69 (25%)	16 (94%)	1 (6%)	0	100	100
3	F	17/69 (25%)	15 (88%)	2 (12%)	0	100	100
All	All	682/822 (83%)	602 (88%)	70 (10%)	10 (2%)	10	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	D	22	THR
2	B	81	CYS
2	B	130	GLU
2	E	81	CYS
1	A	72	ILE
2	E	131	LEU
1	D	72	ILE
2	E	123	ALA
2	B	215	ILE

### 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	62/68 (91%)	56 (90%)	6 (10%)	8	25
1	D	62/68 (91%)	56 (90%)	6 (10%)	8	25
2	B	229/232 (99%)	201 (88%)	28 (12%)	5	15
2	E	229/232 (99%)	199 (87%)	30 (13%)	4	12
3	C	19/62 (31%)	17 (90%)	2 (10%)	7	21
3	F	19/62 (31%)	18 (95%)	1 (5%)	22	54
All	All	620/724 (86%)	547 (88%)	73 (12%)	5	16

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	60	MET
1	A	63	LEU
1	A	70	ILE
1	A	75	ASP
1	A	85	ASP
2	B	1	MET
2	B	2	LEU
2	B	11	LEU
2	B	20	LYS
2	B	41	ASP
2	B	42	ASP
2	B	44	ARG
2	B	47	LEU
2	B	54	VAL
2	B	55	GLU
2	B	72	LEU
2	B	77	LYS
2	B	88	LEU
2	B	99	ILE
2	B	100	ILE
2	B	137	LEU
2	B	154	LEU
2	B	157	SER
2	B	185	PHE
2	B	188	MET
2	B	189	GLU
2	B	192	GLU
2	B	199	MET
2	B	203	VAL
2	B	229	LEU
2	B	230	SER
2	B	242	LYS
2	B	254	PHE
3	C	1170	ILE
3	C	1173	ILE
1	D	22	THR
1	D	60	MET
1	D	63	LEU
1	D	70	ILE
1	D	75	ASP
1	D	85	ASP
2	E	1	MET

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Mol	Chain	Res	Type
2	E	2	LEU
2	E	11	LEU
2	E	41	ASP
2	E	42	ASP
2	E	44	ARG
2	E	47	LEU
2	E	48	VAL
2	E	54	VAL
2	E	55	GLU
2	E	61	ARG
2	E	66	VAL
2	E	72	LEU
2	E	77	LYS
2	E	88	LEU
2	E	99	ILE
2	E	128	ILE
2	E	154	LEU
2	E	156	ASP
2	E	166	THR
2	E	182	ILE
2	E	185	PHE
2	E	188	MET
2	E	192	GLU
2	E	195	ILE
2	E	203	VAL
2	E	205	LEU
2	E	221	LEU
2	E	242	LYS
2	E	254	PHE
3	F	1173	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	86	ASN
1	D	56	GLN
1	D	76	GLN
1	D	86	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	MLY	A	40	1	9,10,11	0.56	0	6,11,13	0.41	0
1	MLY	D	54	1	9,10,11	0.52	0	6,11,13	0.87	0
1	MLY	A	41	1	9,10,11	0.51	0	6,11,13	0.48	0
1	MLY	A	38	1	9,10,11	0.62	0	6,11,13	0.79	0
1	MLY	D	27	1	9,10,11	0.49	0	6,11,13	1.21	1 (16%)
1	MLY	D	41	1	9,10,11	0.50	0	6,11,13	0.50	0
1	MLY	A	58	1	9,10,11	0.65	0	6,11,13	0.79	0
1	MLY	A	27	1	9,10,11	0.53	0	6,11,13	1.28	1 (16%)
1	MLY	D	38	1	9,10,11	0.60	0	6,11,13	0.79	0
1	MLY	A	54	1	9,10,11	0.47	0	6,11,13	0.83	0
1	MLY	D	58	1	9,10,11	0.69	0	6,11,13	0.86	0
1	MLY	D	40	1	9,10,11	0.53	0	6,11,13	0.47	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	MLY	A	40	1	-	3/8/9/11	-
1	MLY	D	54	1	-	1/8/9/11	-
1	MLY	A	41	1	-	4/8/9/11	-
1	MLY	A	38	1	-	2/8/9/11	-
1	MLY	D	27	1	-	1/8/9/11	-
1	MLY	D	41	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	58	1	-	4/8/9/11	-
1	MLY	A	27	1	-	0/8/9/11	-
1	MLY	D	38	1	-	2/8/9/11	-
1	MLY	A	54	1	-	1/8/9/11	-
1	MLY	D	58	1	-	4/8/9/11	-
1	MLY	D	40	1	-	3/8/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	MLY	CD-CE-NZ	-3.09	105.43	113.79
1	D	27	MLY	CD-CE-NZ	-2.88	105.98	113.79

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	40	MLY	N-CA-CB-CG
1	A	40	MLY	C-CA-CB-CG
1	A	41	MLY	C-CA-CB-CG
1	D	41	MLY	C-CA-CB-CG
1	A	58	MLY	C-CA-CB-CG
1	D	58	MLY	C-CA-CB-CG
1	D	40	MLY	N-CA-CB-CG
1	D	40	MLY	C-CA-CB-CG
1	A	41	MLY	CD-CE-NZ-CH2
1	A	38	MLY	CD-CE-NZ-CH2
1	D	41	MLY	CD-CE-NZ-CH1
1	D	41	MLY	CD-CE-NZ-CH2
1	A	40	MLY	CG-CD-CE-NZ
1	D	40	MLY	CG-CD-CE-NZ
1	A	41	MLY	CD-CE-NZ-CH1
1	A	38	MLY	CD-CE-NZ-CH1
1	D	38	MLY	CD-CE-NZ-CH1
1	D	38	MLY	CD-CE-NZ-CH2
1	A	58	MLY	CA-CB-CG-CD
1	D	58	MLY	CE-CD-CG-CB
1	D	58	MLY	CA-CB-CG-CD
1	D	54	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	A	58	MLY	CE-CD-CG-CB
1	A	54	MLY	CE-CD-CG-CB
1	D	58	MLY	CD-CE-NZ-CH1
1	A	41	MLY	N-CA-CB-CG
1	D	41	MLY	N-CA-CB-CG
1	D	27	MLY	CG-CD-CE-NZ
1	A	58	MLY	CD-CE-NZ-CH1

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	41	MLY	1	0
1	A	38	MLY	2	0
1	D	41	MLY	1	0
1	A	58	MLY	1	0
1	D	38	MLY	1	0
1	D	58	MLY	1	0
1	D	40	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
4	NEQ	E	302	2	9,9,9	3.19	3 (33%)	12,12,12	3.31	6 (50%)
4	NEQ	B	302	2	9,9,9	3.17	3 (33%)	12,12,12	3.35	6 (50%)
5	SO4	B	303	-	4,4,4	0.12	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	E	303	-	4,4,4	0.13	0	6,6,6	0.17	0
4	NEQ	B	301	2	9,9,9	3.23	3 (33%)	12,12,12	3.49	6 (50%)
5	SO4	E	304	-	4,4,4	0.14	0	6,6,6	0.12	0
4	NEQ	E	301	2	9,9,9	3.22	4 (44%)	12,12,12	3.65	7 (58%)
5	SO4	B	304	-	4,4,4	0.15	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NEQ	E	302	2	-	0/2/15/15	0/1/1/1
4	NEQ	B	302	2	-	0/2/15/15	0/1/1/1
4	NEQ	B	301	2	-	2/2/15/15	0/1/1/1
4	NEQ	E	301	2	-	2/2/15/15	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	302	NEQ	C3-C2	8.01	1.53	1.35
4	E	301	NEQ	C3-C2	7.92	1.52	1.35
4	B	302	NEQ	C3-C2	7.92	1.52	1.35
4	B	301	NEQ	C3-C2	7.91	1.52	1.35
4	B	301	NEQ	C1-N1	-3.67	1.33	1.40
4	E	301	NEQ	C1-N1	-3.55	1.33	1.40
4	B	302	NEQ	C4-N1	-3.41	1.33	1.40
4	E	302	NEQ	C1-N1	-3.31	1.33	1.40
4	B	302	NEQ	C1-N1	-3.25	1.33	1.40
4	B	301	NEQ	C4-N1	-3.21	1.34	1.40
4	E	302	NEQ	C4-N1	-3.16	1.34	1.40
4	E	301	NEQ	C4-N1	-3.09	1.34	1.40
4	E	301	NEQ	C3-C4	2.09	1.52	1.48

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	301	NEQ	C2-C1-N1	7.39	113.03	106.07
4	B	301	NEQ	C2-C1-N1	7.03	112.69	106.07
4	B	302	NEQ	C3-C4-N1	6.86	112.53	106.07
4	B	301	NEQ	C3-C4-N1	6.83	112.50	106.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	301	NEQ	C3-C4-N1	6.63	112.31	106.07
4	E	302	NEQ	C3-C4-N1	6.55	112.23	106.07
4	E	302	NEQ	C2-C1-N1	6.18	111.89	106.07
4	B	302	NEQ	C2-C1-N1	6.15	111.86	106.07
4	E	302	NEQ	O2-C4-C3	-3.72	121.61	128.56
4	B	301	NEQ	C2-C3-C4	-3.62	102.29	108.67
4	E	301	NEQ	C3-C2-C1	-3.56	102.39	108.67
4	B	302	NEQ	O2-C4-C3	-3.56	121.92	128.56
4	B	302	NEQ	C2-C3-C4	-3.54	102.43	108.67
4	B	301	NEQ	O2-C4-C3	-3.48	122.06	128.56
4	E	302	NEQ	C2-C3-C4	-3.48	102.54	108.67
4	E	301	NEQ	C2-C3-C4	-3.47	102.55	108.67
4	E	301	NEQ	O2-C4-C3	-3.43	122.15	128.56
4	B	301	NEQ	C3-C2-C1	-3.40	102.68	108.67
4	B	302	NEQ	O1-C1-C2	-3.31	122.39	128.56
4	E	302	NEQ	C3-C2-C1	-3.26	102.93	108.67
4	B	302	NEQ	C3-C2-C1	-3.25	102.94	108.67
4	E	301	NEQ	C5-N1-C4	3.20	128.40	123.72
4	E	301	NEQ	O1-C1-C2	-3.16	122.66	128.56
4	E	302	NEQ	O1-C1-C2	-3.14	122.70	128.56
4	B	301	NEQ	O1-C1-C2	-3.12	122.74	128.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	301	NEQ	C6-C5-N1-C1
4	E	301	NEQ	C6-C5-N1-C4
4	B	301	NEQ	C6-C5-N1-C4
4	B	301	NEQ	C6-C5-N1-C1

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, 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	73/84 (86%)	0.45	3 (4%) 37 32	70, 99, 125, 139	0
1	D	73/84 (86%)	0.52	3 (4%) 37 32	72, 98, 128, 137	0
2	B	255/258 (98%)	0.45	6 (2%) 59 56	54, 76, 121, 154	0
2	E	255/258 (98%)	0.44	6 (2%) 59 56	53, 76, 122, 154	0
3	C	21/69 (30%)	1.06	4 (19%) 1 0	92, 120, 139, 163	0
3	F	21/69 (30%)	0.79	1 (4%) 30 27	89, 121, 141, 159	0
All	All	698/822 (84%)	0.48	23 (3%) 46 41	53, 83, 133, 163	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	123	ALA	5.8
2	E	123	ALA	4.2
3	F	1174	ASP	4.2
1	D	20	PRO	4.0
1	A	20	PRO	3.9
3	C	1174	ASP	3.8
2	B	125	PHE	3.3
1	D	98	GLY	3.2
2	B	124	ASP	3.0
3	C	1161	LYS	3.0
2	E	125	PHE	2.9
2	B	129	GLU	2.8
1	A	45	LEU	2.7
3	C	1159	ALA	2.4
2	E	78	ILE	2.3
2	E	124	ASP	2.3
1	D	81	LEU	2.2
1	A	35	ILE	2.2
2	E	52	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	1168	GLY	2.1
2	B	165	GLU	2.1
2	E	243	SER	2.1
2	B	122	ASP	2.0

## 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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	MLY	A	40	11/12	0.85	0.30	109,119,136,137	0
1	MLY	A	38	11/12	0.90	0.38	91,100,124,124	0
1	MLY	D	38	11/12	0.93	0.36	95,105,128,130	0
1	MLY	D	40	11/12	0.93	0.23	107,120,142,144	0
1	MLY	D	41	11/12	0.94	0.30	106,112,132,136	0
1	MLY	A	41	11/12	0.94	0.22	103,114,128,131	0
1	MLY	D	58	11/12	0.94	0.22	82,86,96,104	0
1	MLY	D	54	11/12	0.94	0.23	73,80,94,95	0
1	MLY	A	58	11/12	0.96	0.26	80,86,101,109	0
1	MLY	A	54	11/12	0.96	0.31	77,86,95,96	0
1	MLY	D	27	11/12	0.97	0.29	76,83,91,92	0
1	MLY	A	27	11/12	0.97	0.29	75,81,91,93	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	E	304	5/5	0.80	0.19	160,160,160,160	0
5	SO4	B	303	5/5	0.83	0.40	155,155,156,156	0

*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	E	303	5/5	0.84	0.24	142,142,142,142	0
5	SO4	B	304	5/5	0.87	0.14	165,165,166,166	0
4	NEQ	B	302	9/9	0.90	0.53	119,138,143,143	0
4	NEQ	B	301	9/9	0.92	0.39	87,100,106,108	0
4	NEQ	E	302	9/9	0.92	0.49	117,127,132,133	0
4	NEQ	E	301	9/9	0.95	0.32	82,104,113,115	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.