



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:06 am BST

PDB ID : 5BTR  
Title : Crystal structure of SIRT1 in complex with resveratrol and an AMC-containing peptide  
Authors : Cao, D.; Wang, M.; Qiu, X.; Liu, D.; Jiang, H.; Yang, N.; Xu, R.M.  
Deposited on : 2015-06-03  
Resolution : 3.20 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 : 2.11  
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) : 2.11

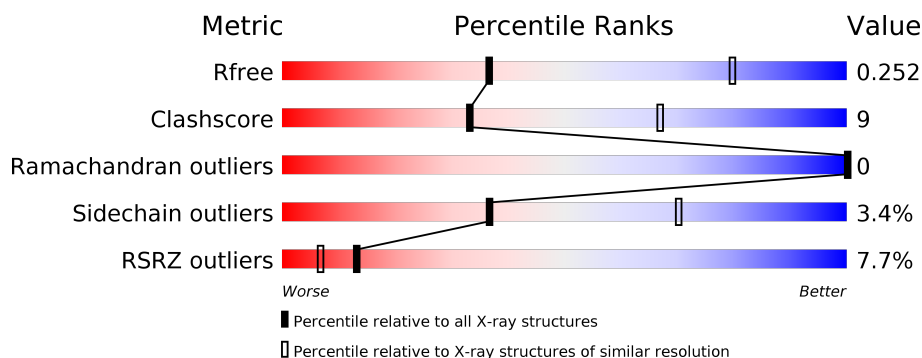
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	397	<div> <div></div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	B	397	<div> <div></div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 8%</div> </div> </div>
1	C	397	<div> <div>20%</div> <div> <div></div> <div>57%</div> <div>23%</div> <div>• 19%</div> </div> </div>
2	D	5	<div> <div></div> <div> <div></div> <div>60%</div> <div>40%</div> </div> </div>
2	E	5	<div> <div></div> <div> <div></div> <div>40%</div> <div>60%</div> </div> </div>
2	F	5	<div> <div></div> <div> <div></div> <div>40%</div> <div>60%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	STL	C	702	-	-	-	X
4	STL	C	703	-	-	-	X
4	STL	F	101	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8800 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 NAD-dependent protein deacetylase sirtuin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2951	1900	498	539	14			
1	B	366	Total	C	N	O	S	0	0	0
			2916	1879	490	533	14			
1	C	322	Total	C	N	O	S	0	0	0
			2592	1679	434	466	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	GLY	-	expression tag	UNP Q96EB6
A	142	SER	-	expression tag	UNP Q96EB6
A	253	SER	CYS	engineered mutation	UNP Q96EB6
A	268	SER	CYS	engineered mutation	UNP Q96EB6
A	501	SER	CYS	engineered mutation	UNP Q96EB6
A	502	SER	CYS	engineered mutation	UNP Q96EB6
B	141	GLY	-	expression tag	UNP Q96EB6
B	142	SER	-	expression tag	UNP Q96EB6
B	253	SER	CYS	engineered mutation	UNP Q96EB6
B	268	SER	CYS	engineered mutation	UNP Q96EB6
B	501	SER	CYS	engineered mutation	UNP Q96EB6
B	502	SER	CYS	engineered mutation	UNP Q96EB6
C	141	GLY	-	expression tag	UNP Q96EB6
C	142	SER	-	expression tag	UNP Q96EB6
C	253	SER	CYS	engineered mutation	UNP Q96EB6
C	268	SER	CYS	engineered mutation	UNP Q96EB6
C	501	SER	CYS	engineered mutation	UNP Q96EB6
C	630	SER	CYS	engineered mutation	UNP Q96EB6

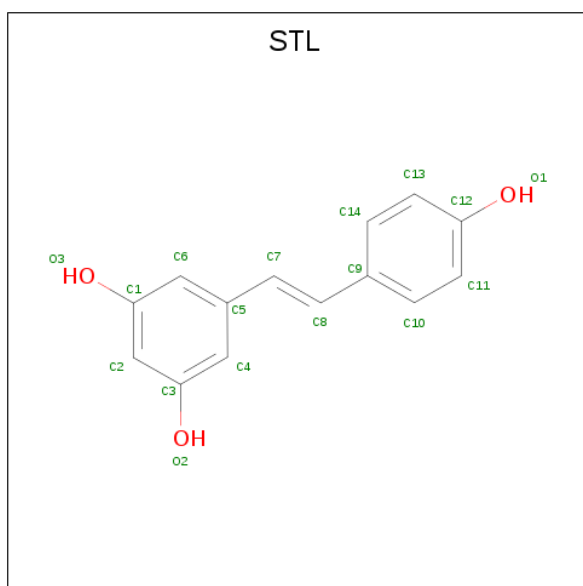
- Molecule 2 is a protein called AMC-containing peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	5	Total	C	N	O	0	0	0
			58	38	12	8			
2	E	5	Total	C	N	O	0	0	0
			58	38	12	8			
2	F	5	Total	C	N	O	0	0	0
			58	38	12	8			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is RESVERATROL (three-letter code: STL) (formula: C<sub>14</sub>H<sub>12</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	14	3		
4	B	1	Total	C	O	0	0
			17	14	3		
4	B	1	Total	C	O	0	0
			17	14	3		
4	C	1	Total	C	O	0	0
			17	14	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			17	14	3		
4	D	1	Total	C	O	0	0
			17	14	3		
4	D	1	Total	C	O	0	0
			17	14	3		
4	E	1	Total	C	O	0	0
			17	14	3		
4	F	1	Total	C	O	0	0
			17	14	3		

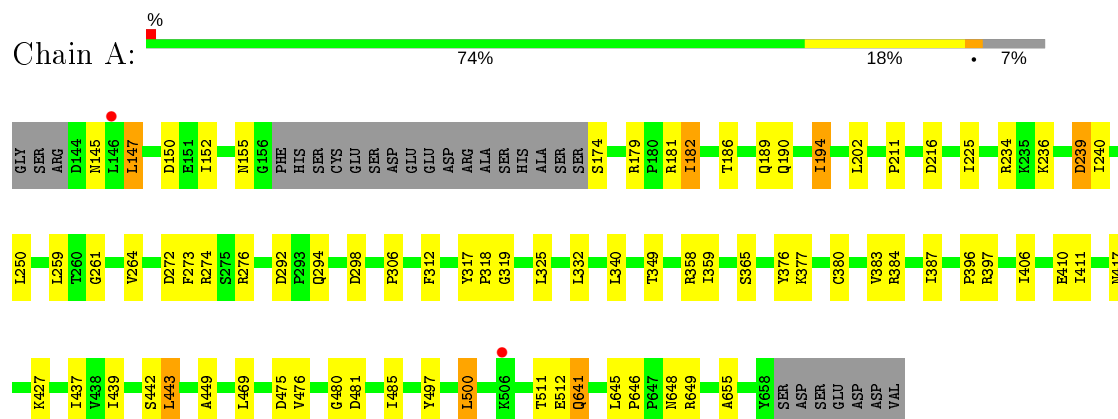
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	3	Total	O	0	0
			3	3		
5	E	1	Total	O	0	0
			1	1		

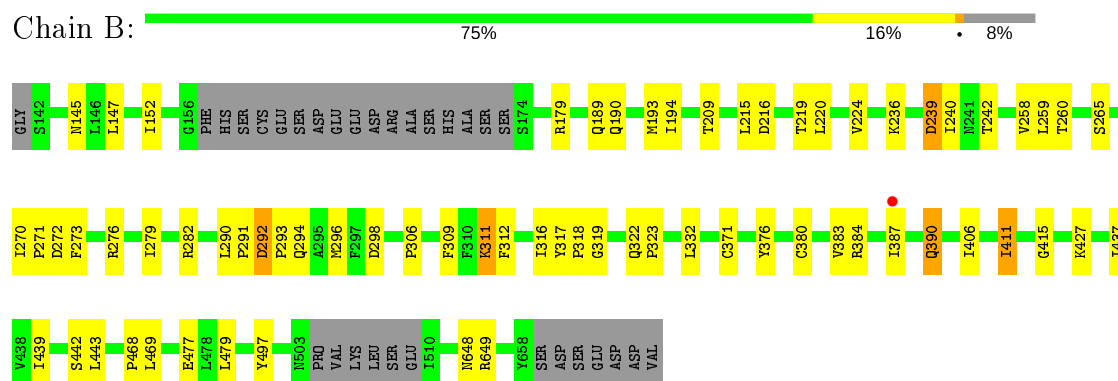
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

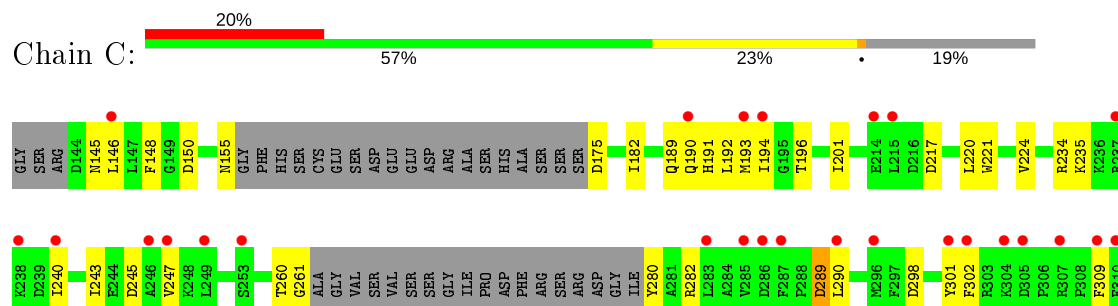
- Molecule 1: NAD-dependent protein deacetylase sirtuin-1

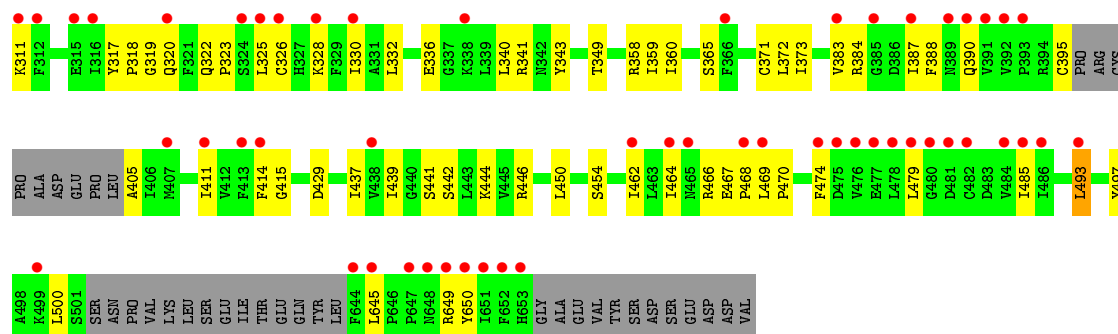


- Molecule 1: NAD-dependent protein deacetylase sirtuin-1



- Molecule 1: NAD-dependent protein deacetylase sirtuin-1





- Molecule 2: AMC-containing peptide

Chain D: 60% 40%



- Molecule 2: AMC-containing peptide

Chain E: 40% 60%



- Molecule 2: AMC-containing peptide

Chain F: 40% 60%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.89Å 133.89Å 106.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.63 – 3.20 46.48 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.63-3.20) 99.8 (46.48-3.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, $R_{free}$	0.207 , 0.252 0.207 , 0.252	Depositor DCC
$R_{free}$ test set	1602 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	102.9	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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

### 5.1 Standard geometry

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

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	0.33	0/3024	0.54	1/4109 (0.0%)
1	B	0.33	0/2988	0.52	0/4060
1	C	0.26	0/2655	0.46	0/3603
2	D	0.51	0/31	0.61	0/39
2	E	0.29	0/31	0.73	0/39
2	F	0.33	0/31	0.64	0/39
All	All	0.31	0/8760	0.51	1/11889 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	LEU	N-CA-C	5.11	124.80	111.00

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	2951	0	2961	47	0
1	B	2916	0	2910	44	0
1	C	2592	0	2602	60	0
2	D	58	0	57	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	58	0	57	3	0
2	F	58	0	57	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	17	0	12	4	0
4	B	34	0	24	4	0
4	C	34	0	24	3	0
4	D	34	0	24	1	0
4	E	17	0	12	0	0
4	F	17	0	12	0	0
5	A	7	0	0	0	0
5	B	3	0	0	0	0
5	E	1	0	0	0	0
All	All	8800	0	8752	151	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 9.

All (151) 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:A:319:GLY:HA3	1:A:384:ARG:HH12	1.39	0.85
1:A:276:ARG:HH21	1:A:292:ASP:HB3	1.46	0.80
1:A:189:GLN:NE2	1:C:193:MET:SD	2.55	0.79
1:A:511:THR:HG22	1:A:641:GLN:H	1.46	0.79
1:B:319:GLY:HA3	1:B:384:ARG:HH12	1.47	0.79
1:A:340:LEU:O	1:A:358:ARG:NH2	2.20	0.73
1:B:147:LEU:HG	1:B:190:GLN:HG2	1.69	0.73
1:B:265:SER:HB3	1:B:270:ILE:HD12	1.70	0.73
1:C:340:LEU:O	1:C:358:ARG:NH2	2.22	0.72
1:B:276:ARG:HH21	1:B:292:ASP:HB3	1.56	0.71
1:C:145:ASN:HD22	1:C:194:ILE:HD11	1.58	0.69
1:B:145:ASN:HB2	1:B:190:GLN:HG3	1.75	0.68
1:C:319:GLY:HA3	1:C:384:ARG:HH12	1.59	0.67
1:A:294:GLN:HG2	4:A:702:STL:H8	1.77	0.66
1:C:373:ILE:HD12	1:C:405:ALA:HB2	1.78	0.65
1:C:383:VAL:HG12	1:C:387:ILE:HG13	1.79	0.65
1:C:466:ARG:HG3	1:C:467:GLU:HG3	1.80	0.64
1:A:239:ASP:HB2	1:A:240:ILE:HD12	1.80	0.63
1:C:289:ASP:OD1	1:C:289:ASP:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LYS:HD2	1:B:648:ASN:HD21	1.65	0.61
1:A:349:THR:HG22	1:A:365:SER:HB2	1.83	0.60
1:B:309:PHE:CZ	1:B:411:ILE:HD11	2.38	0.58
1:C:194:ILE:HB	1:C:196:THR:HG23	1.86	0.58
1:A:152:ILE:HD11	1:A:181:ARG:HE	1.68	0.57
1:C:234:ARG:NH1	1:C:235:LYS:O	2.34	0.57
1:C:243:ILE:N	1:C:650:TYR:OH	2.37	0.57
1:C:442:SER:HB2	1:C:444:LYS:HD3	1.87	0.57
1:A:442:SER:HA	1:A:469:LEU:HD21	1.87	0.57
2:F:1:ARG:HG2	2:F:2:HIS:CE1	2.39	0.56
1:B:193:MET:SD	1:C:189:GLN:NE2	2.73	0.56
1:B:145:ASN:ND2	1:B:194:ILE:HD11	2.21	0.56
4:C:703:STL:H6	2:F:4:FDL:H7	1.88	0.56
1:A:236:LYS:HD2	1:A:648:ASN:HD21	1.70	0.56
1:C:217:ASP:HA	1:C:220:LEU:HD12	1.88	0.56
1:C:450:LEU:O	1:C:454:SER:OG	2.18	0.54
1:B:383:VAL:HG12	1:B:387:ILE:HG13	1.90	0.54
1:B:477:GLU:OE1	1:B:649:ARG:NH2	2.35	0.53
1:C:437:ILE:HG12	1:C:462:ILE:HB	1.89	0.53
1:B:311:LYS:HD2	1:B:390:GLN:HG2	1.90	0.53
1:B:279:ILE:HA	1:B:282:ARG:NH1	2.23	0.53
1:B:152:ILE:HD11	1:B:179:ARG:HH21	1.74	0.52
1:B:215:LEU:HD22	1:B:219:THR:HG21	1.91	0.52
1:C:298:ASP:OD2	4:C:702:STL:O2	2.22	0.52
1:A:145:ASN:ND2	1:A:147:LEU:HD12	2.25	0.52
1:C:309:PHE:CE1	1:C:411:ILE:HD11	2.45	0.51
1:B:294:GLN:HG2	4:B:702:STL:H8	1.93	0.51
1:B:298:ASP:OD2	4:B:702:STL:O2	2.24	0.50
1:C:446:ARG:H	2:F:4:FDL:H5	1.75	0.50
1:B:279:ILE:HA	1:B:282:ARG:HH11	1.77	0.50
1:A:383:VAL:HG12	1:A:387:ILE:HG13	1.94	0.50
1:A:182:ILE:HG22	1:A:186:THR:HB	1.93	0.49
1:A:306:PRO:HG3	1:A:406:ILE:HD13	1.94	0.49
1:B:415:GLY:O	2:E:3:LYS:HD3	2.13	0.49
1:B:239:ASP:HB2	1:B:240:ILE:HD12	1.95	0.49
1:C:415:GLY:HA2	4:C:703:STL:H7	1.93	0.49
1:A:225:ILE:HD11	1:C:146:LEU:HG	1.94	0.49
1:C:317:TYR:CG	1:C:318:PRO:HD2	2.48	0.49
1:C:323:PRO:HB2	1:C:328:LYS:HE3	1.95	0.49
1:B:309:PHE:HZ	1:B:411:ILE:HD11	1.77	0.48
1:A:189:GLN:HE21	1:C:190:GLN:NE2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD23	1:A:211:PRO:HG3	1.95	0.48
1:C:326:CYS:O	1:C:330:ILE:HG13	2.14	0.48
1:B:220:LEU:O	1:B:224:VAL:HG23	2.14	0.48
1:A:317:TYR:CD2	1:A:318:PRO:HD2	2.49	0.47
1:B:279:ILE:HD13	1:B:282:ARG:NH1	2.29	0.47
1:A:150:ASP:OD1	2:E:1:ARG:NH1	2.47	0.47
1:C:260:THR:HG22	1:C:439:ILE:HB	1.97	0.47
1:A:261:GLY:O	1:A:264:VAL:HG22	2.15	0.47
1:C:240:ILE:HD12	1:C:245:ASP:HB3	1.97	0.47
1:A:427:LYS:HD2	1:C:175:ASP:OD2	2.16	0.46
1:C:332:LEU:O	1:C:336:GLU:HG3	2.15	0.46
1:C:247:VAL:HG13	1:C:493:LEU:HD12	1.97	0.46
1:C:261:GLY:HA3	1:C:441:SER:HB2	1.98	0.46
1:C:317:TYR:CD2	1:C:318:PRO:HD2	2.50	0.46
1:C:311:LYS:HD2	1:C:390:GLN:HG2	1.97	0.46
1:A:376:TYR:HB2	1:A:397:ARG:HH21	1.81	0.45
1:B:317:TYR:CD2	1:B:318:PRO:HD2	2.51	0.45
1:A:190:GLN:O	1:A:194:ILE:HG13	2.16	0.45
1:B:272:ASP:OD1	1:B:272:ASP:N	2.46	0.45
4:B:702:STL:H13	2:E:4:FDL:CAB	2.46	0.45
1:A:240:ILE:HG22	1:A:476:VAL:HG23	1.98	0.45
1:B:258:VAL:HG12	1:B:260:THR:HG23	1.98	0.45
1:A:376:TYR:CE2	1:A:396:PRO:HG2	2.52	0.45
1:C:493:LEU:HD23	1:C:497:TYR:CD1	2.51	0.45
1:A:417:ASN:OD1	2:D:3:LYS:HG2	2.17	0.45
1:C:645:LEU:HB2	1:C:649:ARG:HB3	1.99	0.44
1:B:145:ASN:CG	1:B:194:ILE:HD11	2.38	0.44
1:C:145:ASN:ND2	1:C:194:ILE:HD11	2.29	0.44
1:C:469:LEU:HA	1:C:470:PRO:HD3	1.80	0.44
1:A:377:LYS:HE3	1:A:410:GLU:OE1	2.17	0.44
1:C:148:PHE:HB3	1:C:150:ASP:OD1	2.17	0.44
1:C:220:LEU:O	1:C:224:VAL:HG23	2.18	0.44
1:B:319:GLY:HA3	1:B:384:ARG:NH1	2.25	0.43
1:C:371:CYS:SG	1:C:395:CYS:HB2	2.57	0.43
1:C:191:HIS:O	1:C:196:THR:OG1	2.36	0.43
1:C:349:THR:HG22	1:C:365:SER:HB2	2.00	0.43
1:C:320:GLN:HE22	1:C:388:PHE:HZ	1.67	0.43
4:A:702:STL:H7	2:D:4:FDL:H2	2.00	0.43
1:A:189:GLN:HE21	1:C:190:GLN:HE22	1.67	0.43
1:B:468:PRO:HG3	1:B:479:LEU:HD13	2.01	0.43
1:C:469:LEU:HB2	1:C:474:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:TYR:HE1	1:C:290:LEU:HB3	1.84	0.43
1:C:302:PHE:HE1	1:C:372:LEU:HD11	1.83	0.43
1:C:309:PHE:HE1	1:C:411:ILE:HD11	1.84	0.43
1:A:298:ASP:OD2	4:A:702:STL:O3	2.26	0.43
1:B:270:ILE:HA	1:B:271:PRO:HD2	1.76	0.43
1:B:306:PRO:HG3	1:B:406:ILE:HD13	2.01	0.42
1:C:189:GLN:O	1:C:192:LEU:HB2	2.19	0.42
1:B:442:SER:HA	1:B:469:LEU:HD21	2.01	0.42
1:A:332:LEU:HD23	1:A:497:TYR:CD1	2.55	0.42
1:A:645:LEU:HA	1:A:646:PRO:HD2	1.78	0.42
1:C:468:PRO:HG3	1:C:479:LEU:HD13	2.01	0.42
1:B:332:LEU:HD23	1:B:497:TYR:CD1	2.55	0.42
1:C:343:TYR:OH	1:C:429:ASP:OD1	2.26	0.42
1:A:437:ILE:HG22	1:A:439:ILE:HG13	2.01	0.42
1:B:309:PHE:CE1	1:B:411:ILE:HD11	2.55	0.42
1:C:282:ARG:H	1:C:282:ARG:HG3	1.57	0.42
2:D:3:LYS:HB2	4:D:102:STL:C10	2.50	0.42
2:F:4:FDL:H1	2:F:4:FDL:H6	1.98	0.41
1:A:294:GLN:HG2	4:A:702:STL:C8	2.48	0.41
1:A:480:GLY:HA2	1:A:655:ALA:CA	2.50	0.41
1:A:645:LEU:HB2	1:A:649:ARG:HB3	2.02	0.41
1:C:201:ILE:HD12	1:C:221:TRP:CZ3	2.56	0.41
1:A:497:TYR:O	1:A:500:LEU:HB2	2.20	0.41
1:A:273:PHE:HE1	1:A:274:ARG:HE	1.66	0.41
1:C:341:ARG:HD2	1:C:360:ILE:HG12	2.03	0.41
1:B:371:CYS:HB3	1:B:376:TYR:H	1.86	0.41
1:C:500:LEU:HD23	1:C:500:LEU:HA	1.83	0.41
1:C:290:LEU:HD23	1:C:301:TYR:HE2	1.86	0.41
1:A:411:ILE:HG12	1:A:411:ILE:H	1.75	0.41
1:B:273:PHE:HB3	1:B:312:PHE:CE1	2.56	0.41
1:A:174:SER:HA	1:B:427:LYS:HD2	2.02	0.41
1:A:234:ARG:HH22	1:A:475:ASP:CG	2.24	0.41
1:B:290:LEU:HA	1:B:291:PRO:HD3	1.86	0.41
1:B:293:PRO:O	1:B:296:MET:HB2	2.21	0.41
1:C:414:PHE:CD1	2:F:4:FDL:H17	2.56	0.41
1:A:272:ASP:OD1	1:A:272:ASP:N	2.51	0.40
1:B:322:GLN:HA	1:B:323:PRO:HD3	1.93	0.40
1:B:437:ILE:HG22	1:B:439:ILE:HG13	2.04	0.40
1:B:479:LEU:HD11	1:B:649:ARG:HD2	2.03	0.40
1:A:250:LEU:HD11	1:A:437:ILE:HD11	2.03	0.40
1:A:443:LEU:HG	1:A:449:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PRO:HG2	1:B:316:ILE:HG22	2.03	0.40
1:C:289:ASP:HB2	1:C:301:TYR:OH	2.21	0.40
1:C:322:GLN:HA	1:C:323:PRO:HD3	1.97	0.40
1:A:150:ASP:O	1:A:179:ARG:HD3	2.21	0.40
1:A:194:ILE:H	1:A:194:ILE:HG13	1.66	0.40
1:A:481:ASP:O	1:A:485:ILE:HG13	2.22	0.40
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.85	0.40
4:B:702:STL:H4	4:B:703:STL:O3	2.22	0.40
1:C:464:ILE:HG23	1:C:485:ILE:HD12	2.04	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	366/397 (92%)	355 (97%)	11 (3%)	0	100	100
1	B	360/397 (91%)	351 (98%)	9 (2%)	0	100	100
1	C	312/397 (79%)	306 (98%)	6 (2%)	0	100	100
2	D	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
2	E	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
2	F	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	1047/1206 (87%)	1018 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/358 (92%)	317 (96%)	14 (4%)	30	65
1	B	325/358 (91%)	313 (96%)	12 (4%)	34	68
1	C	290/358 (81%)	284 (98%)	6 (2%)	53	79
2	D	3/3 (100%)	3 (100%)	0	100	100
2	E	3/3 (100%)	3 (100%)	0	100	100
2	F	3/3 (100%)	3 (100%)	0	100	100
All	All	955/1083 (88%)	923 (97%)	32 (3%)	37	70

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	155	ASN
1	A	182	ILE
1	A	194	ILE
1	A	216	ASP
1	A	239	ASP
1	A	259	LEU
1	A	312	PHE
1	A	325	LEU
1	A	359	ILE
1	A	380	CYS
1	A	443	LEU
1	A	512	GLU
1	A	641	GLN
1	B	189	GLN
1	B	209	THR
1	B	216	ASP
1	B	239	ASP
1	B	242	THR
1	B	259	LEU
1	B	292	ASP
1	B	311	LYS
1	B	380	CYS
1	B	390	GLN
1	B	411	ILE
1	B	443	LEU
1	C	155	ASN

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Mol	Chain	Res	Type
1	C	182	ILE
1	C	289	ASP
1	C	325	LEU
1	C	359	ILE
1	C	493	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	222	GLN
1	A	352	GLN
1	A	361	GLN
1	A	653	HIS
1	B	190	GLN
1	B	222	GLN
1	B	241	ASN
1	B	361	GLN
1	C	190	GLN
1	C	222	GLN
1	C	352	GLN
1	C	357	GLN
1	C	361	GLN
1	C	491	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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
2	FDL	F	4	2	24,26,26	2.81	10 (41%)	30,35,35	1.29	5 (16%)
2	FDL	D	4	2	24,26,26	2.72	11 (45%)	30,35,35	1.29	4 (13%)
2	FDL	E	4	2	24,26,26	2.70	11 (45%)	30,35,35	1.52	6 (20%)

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	FDL	F	4	2	-	1/16/16/16	0/2/2/2
2	FDL	D	4	2	-	2/16/16/16	0/2/2/2
2	FDL	E	4	2	-	1/16/16/16	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	FDL	C-NAM	6.20	1.49	1.35
2	E	4	FDL	C-NAM	5.78	1.48	1.35
2	D	4	FDL	C-NAM	5.70	1.48	1.35
2	F	4	FDL	CAI-CAJ	5.38	1.48	1.39
2	F	4	FDL	CAH-CAE	5.35	1.53	1.42
2	E	4	FDL	CAI-CAJ	5.26	1.48	1.39
2	D	4	FDL	CAI-CAJ	5.25	1.48	1.39
2	D	4	FDL	CAH-CAE	5.25	1.53	1.42
2	E	4	FDL	CAH-CAE	5.23	1.53	1.42
2	F	4	FDL	CAG-CAF	4.69	1.46	1.37
2	D	4	FDL	CAG-CAF	4.29	1.46	1.37
2	E	4	FDL	CAG-CAF	4.14	1.45	1.37
2	F	4	FDL	CAW-NAV	3.95	1.45	1.34
2	E	4	FDL	CAW-NAV	3.65	1.44	1.34
2	D	4	FDL	CAW-NAV	3.62	1.44	1.34
2	D	4	FDL	CAC-CAD	3.23	1.44	1.39
2	E	4	FDL	CAC-CAD	3.22	1.44	1.39
2	F	4	FDL	CAC-CAD	3.16	1.44	1.39
2	F	4	FDL	CAJ-NAM	2.99	1.47	1.41
2	F	4	FDL	CAG-CAJ	2.92	1.43	1.37
2	D	4	FDL	OAY-CAW	-2.87	1.16	1.23
2	E	4	FDL	CAJ-NAM	2.85	1.47	1.41
2	E	4	FDL	OAY-CAW	-2.84	1.16	1.23
2	D	4	FDL	CAJ-NAM	2.77	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	FDL	OAY-CAW	-2.71	1.17	1.23
2	D	4	FDL	CAE-CAF	-2.57	1.37	1.41
2	E	4	FDL	CAG-CAJ	2.55	1.43	1.37
2	D	4	FDL	CAG-CAJ	2.51	1.43	1.37
2	D	4	FDL	O-C	-2.34	1.18	1.23
2	E	4	FDL	CAE-CAF	-2.30	1.38	1.41
2	E	4	FDL	O-C	-2.18	1.19	1.23
2	F	4	FDL	CAD-CAE	2.11	1.47	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	FDL	CAH-CAE-CAF	3.42	120.46	116.50
2	E	4	FDL	CAG-CAF-CAE	-3.07	119.64	123.05
2	D	4	FDL	CAG-CAF-CAE	-2.94	119.79	123.05
2	E	4	FDL	CAX-CAW-NAV	2.92	121.26	116.09
2	F	4	FDL	CAH-CAE-CAF	2.87	119.83	116.50
2	D	4	FDL	CAH-CAE-CAF	2.84	119.78	116.50
2	F	4	FDL	CAX-CAW-NAV	2.81	121.07	116.09
2	F	4	FDL	CAG-CAF-CAE	-2.75	120.00	123.05
2	E	4	FDL	CAU-NAV-CAW	-2.57	118.60	122.56
2	D	4	FDL	CAX-CAW-NAV	2.50	120.52	116.09
2	E	4	FDL	OAA-CAB-CAC	2.48	122.43	119.27
2	F	4	FDL	OAA-CAB-CAC	2.36	122.28	119.27
2	E	4	FDL	CB-CA-C	-2.24	106.00	110.85
2	F	4	FDL	CAU-NAV-CAW	-2.22	119.14	122.56
2	D	4	FDL	CAU-NAV-CAW	-2.18	119.21	122.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	FDL	CB-CAS-CAT-CAU
2	D	4	FDL	CB-CAS-CAT-CAU
2	F	4	FDL	CB-CAS-CAT-CAU
2	D	4	FDL	CAS-CAT-CAU-NAV

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	4	FDL	4	0
2	D	4	FDL	1	0
2	E	4	FDL	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	STL	D	102	-	18,18,18	0.90	0	24,24,24	0.72	1 (4%)
4	STL	B	703	-	18,18,18	0.95	0	24,24,24	0.53	0
4	STL	A	702	-	18,18,18	0.94	0	24,24,24	0.51	0
4	STL	C	702	-	18,18,18	0.92	0	24,24,24	0.57	0
4	STL	B	702	-	18,18,18	0.88	0	24,24,24	0.85	1 (4%)
4	STL	D	101	-	18,18,18	0.93	0	24,24,24	0.64	0
4	STL	E	101	-	18,18,18	0.95	0	24,24,24	0.73	0
4	STL	F	101	-	18,18,18	0.91	0	24,24,24	0.58	0
4	STL	C	703	-	18,18,18	0.92	0	24,24,24	0.67	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	STL	D	102	-	-	4/5/5/5	0/2/2/2
4	STL	B	703	-	-	2/5/5/5	0/2/2/2
4	STL	A	702	-	-	4/5/5/5	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	STL	C	702	-	-	4/5/5/5	0/2/2/2
4	STL	B	702	-	-	2/5/5/5	0/2/2/2
4	STL	D	101	-	-	2/5/5/5	0/2/2/2
4	STL	E	101	-	-	2/5/5/5	0/2/2/2
4	STL	F	101	-	-	3/5/5/5	0/2/2/2
4	STL	C	703	-	-	4/5/5/5	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	102	STL	C5-C7-C8	-2.08	117.68	125.87
4	B	702	STL	C14-C9-C10	2.05	120.67	117.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	STL	C4-C5-C7-C8
4	A	702	STL	C7-C8-C9-C10
4	C	703	STL	C7-C8-C9-C10
4	C	702	STL	C7-C8-C9-C10
4	F	101	STL	C7-C8-C9-C10
4	C	703	STL	C4-C5-C7-C8
4	D	102	STL	C4-C5-C7-C8
4	C	703	STL	C6-C5-C7-C8
4	F	101	STL	C7-C8-C9-C14
4	C	702	STL	C7-C8-C9-C14
4	A	702	STL	C6-C5-C7-C8
4	A	702	STL	C7-C8-C9-C14
4	C	703	STL	C7-C8-C9-C14
4	D	102	STL	C6-C5-C7-C8
4	C	702	STL	C4-C5-C7-C8
4	B	703	STL	C4-C5-C7-C8
4	C	702	STL	C6-C5-C7-C8
4	B	703	STL	C6-C5-C7-C8
4	B	702	STL	C4-C5-C7-C8
4	B	702	STL	C6-C5-C7-C8
4	D	101	STL	C7-C8-C9-C14
4	D	101	STL	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
4	D	102	STL	C7-C8-C9-C14
4	D	102	STL	C7-C8-C9-C10
4	F	101	STL	C5-C7-C8-C9
4	E	101	STL	C7-C8-C9-C14
4	E	101	STL	C7-C8-C9-C10

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	102	STL	1	0
4	B	703	STL	1	0
4	A	702	STL	4	0
4	C	702	STL	1	0
4	B	702	STL	4	0
4	C	703	STL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	370/397 (93%)	0.08	2 (0%) 91 86	48, 72, 104, 143	0
1	B	366/397 (92%)	0.08	1 (0%) 94 92	47, 74, 119, 149	0
1	C	322/397 (81%)	1.22	79 (24%) 0 0	76, 166, 196, 212	0
2	D	3/5 (60%)	-0.16	0 100 100	67, 67, 78, 83	0
2	E	3/5 (60%)	-0.08	0 100 100	59, 59, 65, 73	0
2	F	3/5 (60%)	-0.23	0 100 100	87, 87, 102, 104	0
All	All	1067/1206 (88%)	0.42	82 (7%) 13 7	47, 82, 187, 212	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	311	LYS	9.0
1	C	476	VAL	8.6
1	C	309	PHE	6.5
1	C	310	PHE	5.7
1	C	480	GLY	5.2
1	C	285	VAL	4.9
1	C	302	PHE	4.9
1	C	246	ALA	4.9
1	C	387	ILE	4.5
1	C	468	PRO	4.5
1	C	652	PHE	4.4
1	C	649	ARG	4.4
1	C	653	HIS	4.3
1	C	478	LEU	4.3
1	C	477	GLU	4.1
1	C	465	ASN	4.0
1	C	469	LEU	4.0
1	C	651	ILE	4.0
1	C	383	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	325	LEU	3.8
1	C	194	ILE	3.8
1	C	389	ASN	3.8
1	C	290	LEU	3.7
1	C	237	ARG	3.5
1	C	240	ILE	3.5
1	C	296	MET	3.5
1	C	481	ASP	3.5
1	C	407	MET	3.3
1	C	644	PHE	3.3
1	C	305	ASP	3.3
1	C	366	PHE	3.3
1	C	474	PHE	3.3
1	C	146	LEU	3.2
1	C	648	ASN	3.2
1	A	506	LYS	3.1
1	C	484	VAL	3.1
1	C	238	LYS	3.0
1	C	312	PHE	3.0
1	C	482	CYS	3.0
1	C	326	CYS	2.9
1	C	390	GLN	2.9
1	C	315	GLU	2.9
1	C	320	GLN	2.9
1	C	316	ILE	2.8
1	C	253	SER	2.8
1	C	283	LEU	2.8
1	C	247	VAL	2.7
1	C	392	VAL	2.7
1	C	338	LYS	2.7
1	C	462	ILE	2.7
1	C	214	GLU	2.6
1	C	301	TYR	2.6
1	C	411	ILE	2.6
1	C	190	GLN	2.6
1	C	650	TYR	2.6
1	C	486	ILE	2.5
1	C	479	LEU	2.5
1	C	249	LEU	2.5
1	C	328	LYS	2.4
1	C	485	ILE	2.4
1	C	307	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	391	VAL	2.4
1	C	438	VAL	2.3
1	C	304	LYS	2.3
1	A	146	LEU	2.3
1	C	464	ILE	2.3
1	C	414	PHE	2.3
1	C	385	GLY	2.2
1	C	475	ASP	2.2
1	C	393	PRO	2.2
1	C	493	LEU	2.2
1	C	645	LEU	2.1
1	C	499	LYS	2.1
1	C	215	LEU	2.1
1	C	286	ASP	2.1
1	C	647	PRO	2.1
1	C	287	PHE	2.1
1	C	330	ILE	2.1
1	C	324	SER	2.1
1	C	413	PHE	2.1
1	B	387	ILE	2.0
1	C	193	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
2	FDL	F	4	25/25	0.84	0.34	108,125,143,144	0
2	FDL	D	4	25/25	0.96	0.28	50,58,67,73	0
2	FDL	E	4	25/25	0.97	0.26	44,55,58,64	0

## 6.3 Carbohydrates [i](#)

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. 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
4	STL	C	702	17/17	0.58	0.91	127,143,157,159	0
3	ZN	C	701	1/1	0.64	0.07	185,185,185,185	0
4	STL	C	703	17/17	0.71	1.06	91,117,130,130	0
4	STL	F	101	17/17	0.80	0.55	102,108,125,125	0
4	STL	A	702	17/17	0.93	0.40	55,59,66,70	0
4	STL	B	703	17/17	0.94	0.27	46,51,71,86	0
4	STL	D	102	17/17	0.94	0.39	57,62,68,77	0
4	STL	D	101	17/17	0.94	0.40	47,52,63,66	0
3	ZN	B	701	1/1	0.95	0.13	113,113,113,113	0
4	STL	B	702	17/17	0.96	0.22	52,60,66,66	0
3	ZN	A	701	1/1	0.97	0.19	64,64,64,64	0
4	STL	E	101	17/17	0.98	0.31	48,55,62,65	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.