



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:50 AM GMT

PDB ID : 3Q4J  
Title : Structure of a small peptide ligand bound to E.coli DNA sliding clamp  
Authors : Wolff, P.; Olieric, V.; Briand, J.P.; Chaloin, O.; Dejaegere, A.; Dumas, P.;  
Ennifar, E.; Guichard, G.; Wagner, J.; Burnouf, D.  
Deposited on : 2010-12-23  
Resolution : 2.30 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

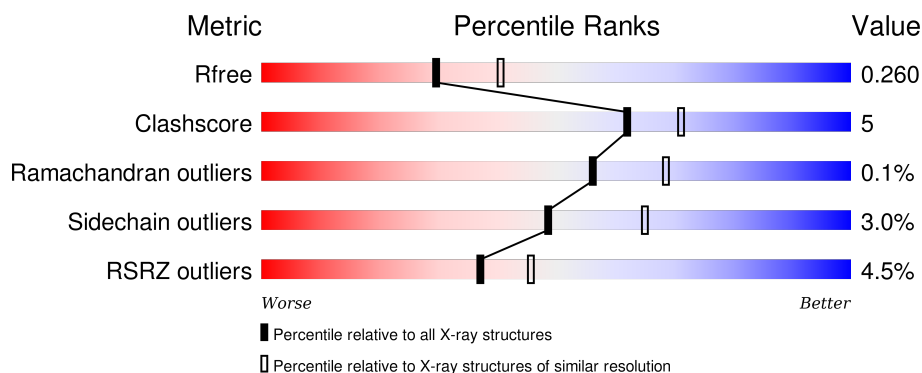
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	366	<div> <div>5%</div> <div>84%</div> <div>16%</div> </div>
1	B	366	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	C	366	<div> <div>6%</div> <div>85%</div> <div>15%</div> </div>
1	D	366	<div> <div>4%</div> <div>81%</div> <div>19%</div> </div>
1	E	366	<div> <div>4%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	366	<div><div></div><div>3%</div><div>85%</div><div>15%</div></div>
2	H	6	<div><div></div><div>67%</div><div>33%</div></div>
2	I	6	<div><div></div><div>50%</div><div>83%</div><div>17%</div></div>
2	J	6	<div><div></div><div>50%</div><div>67%</div><div>33%</div></div>
2	K	6	<div><div></div><div>67%</div><div>33%</div></div>
2	L	6	<div><div></div><div>50%</div><div>50%</div><div>50%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17322 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 DNA polymerase III subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	1	0
			2774	1747	479	530	18			
1	B	364	Total	C	N	O	S	0	0	0
			2792	1756	485	532	19			
1	C	365	Total	C	N	O	S	0	0	0
			2772	1748	472	533	19			
1	D	365	Total	C	N	O	S	0	0	0
			2779	1748	482	530	19			
1	E	364	Total	C	N	O	S	0	0	0
			2777	1744	482	532	19			
1	F	365	Total	C	N	O	S	0	0	0
			2800	1762	486	533	19			

- Molecule 2 is a protein called peptide ligand.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	6	Total	C	N	O	0	0	0
			48	32	6	10			
2	I	6	Total	C	N	O	0	0	0
			48	32	6	10			
2	J	6	Total	C	N	O	0	0	0
			48	32	6	10			
2	K	6	Total	C	N	O	0	0	0
			48	32	6	10			
2	L	6	Total	C	N	O	0	0	0
			48	32	6	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		

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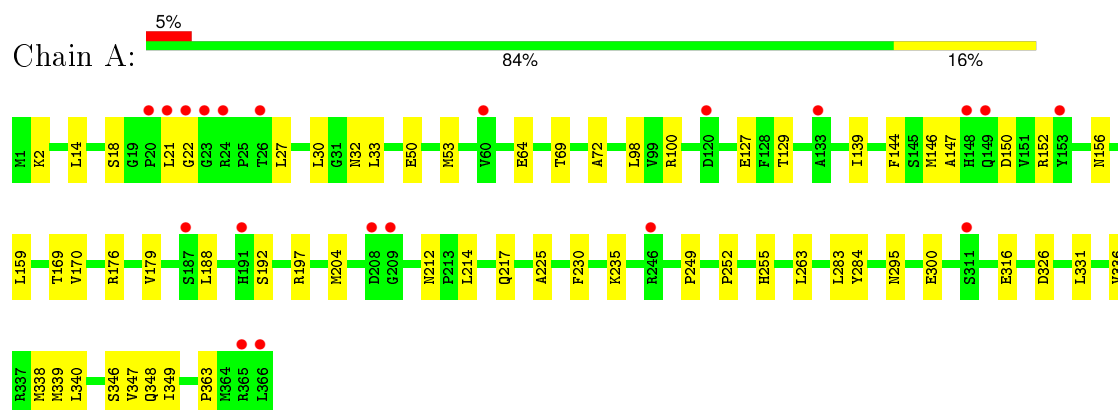
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	98	Total 98	O 98	0	0
3	C	44	Total 44	O 44	0	0
3	D	46	Total 46	O 46	0	0
3	E	75	Total 75	O 75	0	0
3	F	72	Total 72	O 72	0	0
3	H	3	Total 3	O 3	0	0
3	K	2	Total 2	O 2	0	0

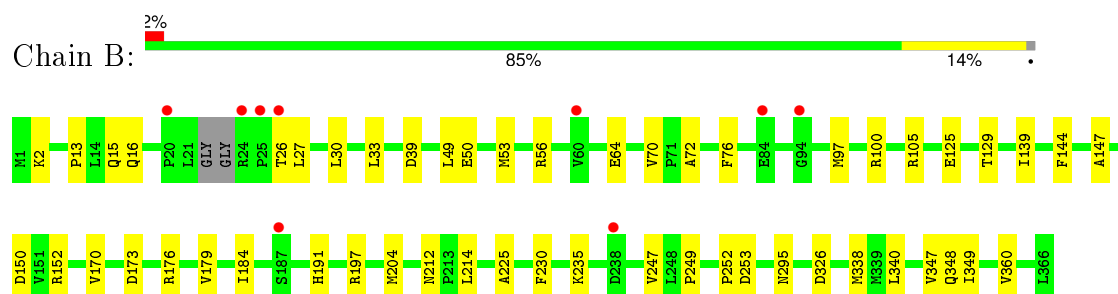
### 3 Residue-property plots [i](#)

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

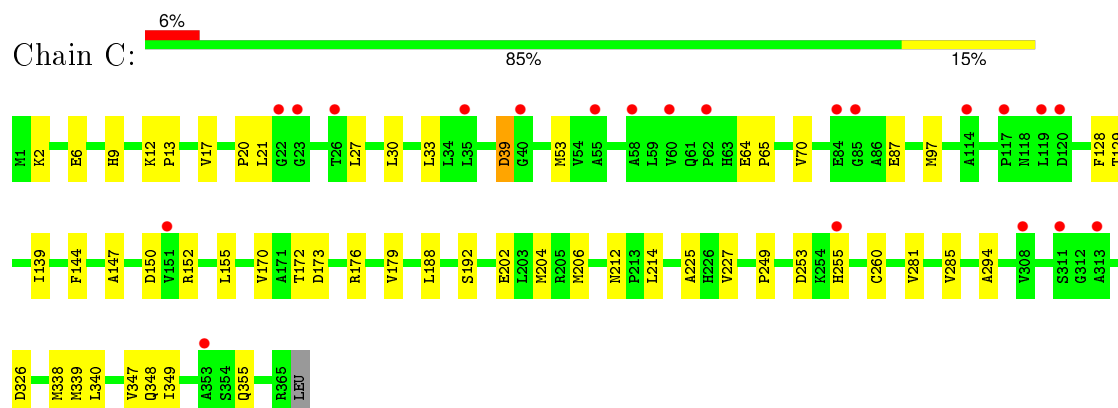
- Molecule 1: DNA polymerase III subunit beta



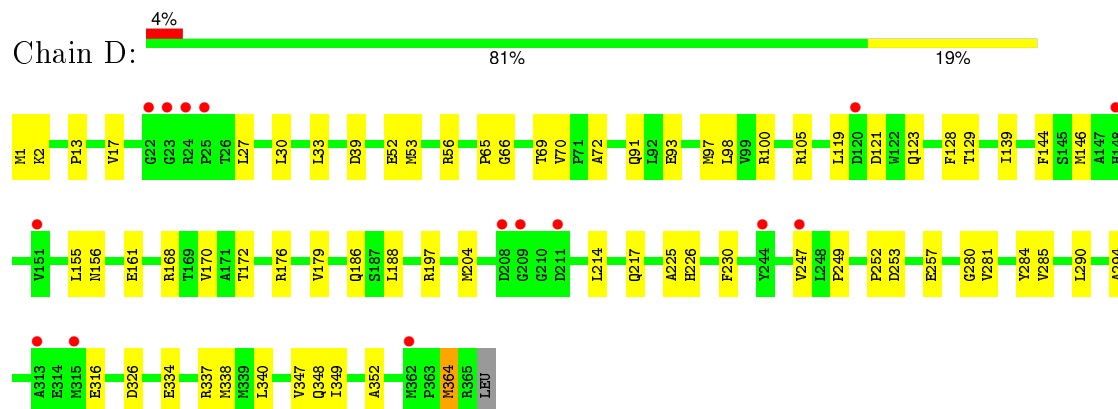
- Molecule 1: DNA polymerase III subunit beta



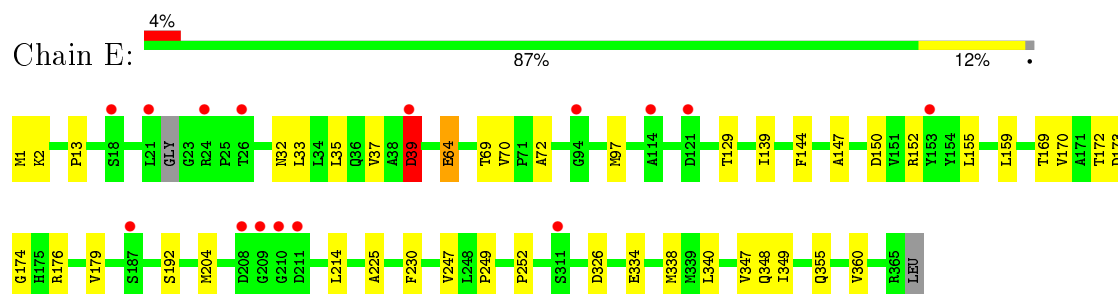
- Molecule 1: DNA polymerase III subunit beta



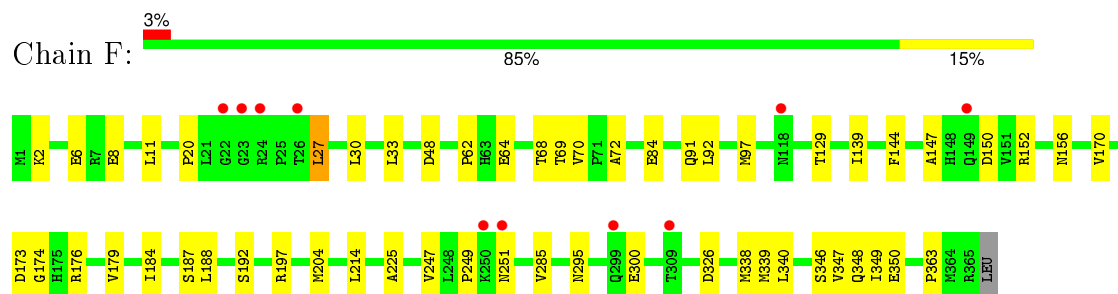
- Molecule 1: DNA polymerase III subunit beta



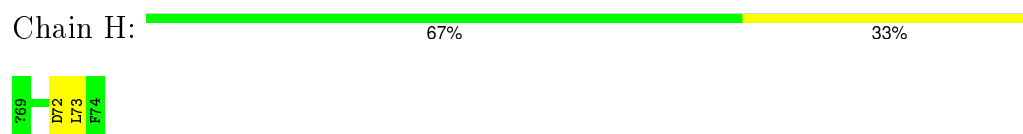
- Molecule 1: DNA polymerase III subunit beta



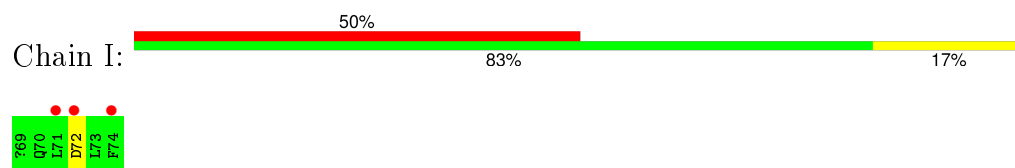
- Molecule 1: DNA polymerase III subunit beta



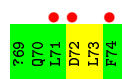
- Molecule 2: peptide ligand



- Molecule 2: peptide ligand



- Molecule 2: peptide ligand



- Molecule 2: peptide ligand



- Molecule 2: peptide ligand





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	35.09Å 132.87Å 137.27Å 62.73° 88.51° 89.77°	Depositor
Resolution (Å)	29.52 – 2.30 29.52 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.52-2.30) 82.6 (29.52-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.50 (at 2.31Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.214 , 0.254 0.220 , 0.260	Depositor DCC
$R_{free}$ test set	1959 reflections (2.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.1	EDS
Estimated twinning fraction	0.024 for h,-k,-l 0.000 for -h,k,k-l 0.000 for -h,-k,-k+l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 96503 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.46	0/2827	0.69	0/3841
1	B	0.53	0/2840	0.70	0/3851
1	C	0.49	0/2821	0.73	0/3829
1	D	0.48	0/2826	0.70	0/3837
1	E	0.51	0/2825	0.70	1/3831 (0.0%)
1	F	0.53	0/2847	0.72	0/3860
2	H	0.69	0/46	0.70	0/60
2	I	0.58	0/46	0.67	0/60
2	J	0.55	0/46	0.67	0/60
2	K	0.57	0/46	0.65	0/60
2	L	0.56	0/46	0.61	0/60
All	All	0.50	0/17216	0.70	1/23349 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	E	39	ASP	N-CA-C	5.75	126.51	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	2774	0	2722	35	0
1	B	2792	0	2771	27	0
1	C	2772	0	2731	26	0
1	D	2779	0	2738	41	0
1	E	2777	0	2726	27	0
1	F	2800	0	2789	27	0
2	H	48	0	46	2	0
2	I	48	0	46	0	0
2	J	48	0	46	1	0
2	K	48	0	46	3	0
2	L	48	0	46	2	0
3	A	48	0	0	0	0
3	B	98	0	0	0	0
3	C	44	0	0	1	0
3	D	46	0	0	0	0
3	E	75	0	0	0	0
3	F	72	0	0	0	0
3	H	3	0	0	0	0
3	K	2	0	0	0	0
All	All	17322	0	16707	180	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 5.

All (180) 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:32:ASN:HB3	1:A:69:THR:HG22	1.28	1.13
1:D:280:GLY:HA2	1:D:364:MET:HE1	1.35	1.09
1:E:32:ASN:HB3	1:E:69:THR:HG22	1.33	1.05
1:D:280:GLY:CA	1:D:364:MET:HE1	1.98	0.91
1:D:1:MET:HB3	1:D:66:GLY:HA3	1.57	0.86
1:C:260:CYS:SG	3:C:415:HOH:O	2.42	0.77
1:A:127:GLU:HB2	1:C:65:PRO:HG3	1.70	0.73
1:A:32:ASN:CB	1:A:69:THR:HG22	2.14	0.73
1:D:280:GLY:HA2	1:D:364:MET:CE	2.15	0.73
1:A:98:LEU:HD23	1:A:100:ARG:HH12	1.50	0.72
1:E:249:PRO:HD2	1:E:348:GLN:HE21	1.54	0.71
1:F:2:LYS:HB2	1:F:64:GLU:HB2	1.73	0.70
1:A:249:PRO:HD2	1:A:348:GLN:HE21	1.56	0.70
1:B:249:PRO:HD2	1:B:348:GLN:HE21	1.57	0.69
1:B:16:GLN:HE21	1:B:53:MET:HE2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LEU:HD11	1:C:225:ALA:HB1	1.75	0.68
1:E:214:LEU:HD11	1:E:225:ALA:HB1	1.76	0.67
1:C:249:PRO:HD2	1:C:348:GLN:HE21	1.58	0.67
1:E:1:MET:HE2	1:E:37:VAL:HG23	1.77	0.67
1:E:32:ASN:CB	1:E:69:THR:HG22	2.19	0.66
1:D:214:LEU:HD11	1:D:225:ALA:HB1	1.77	0.66
1:D:98:LEU:HD23	1:D:100:ARG:HH12	1.59	0.66
1:A:249:PRO:HB2	1:A:252:PRO:HG3	1.78	0.66
1:F:139:ILE:HG21	1:F:204:MET:HG2	1.76	0.66
1:A:214:LEU:HD11	1:A:225:ALA:HB1	1.78	0.65
1:B:100:ARG:HG2	1:B:105:ARG:HG2	1.78	0.65
1:D:1:MET:HB3	1:D:66:GLY:CA	2.26	0.65
1:C:338:MET:HG2	1:C:349:ILE:HG12	1.79	0.65
1:D:249:PRO:HD2	1:D:348:GLN:HE21	1.62	0.64
1:F:214:LEU:HD11	1:F:225:ALA:HB1	1.80	0.63
1:B:53:MET:HE3	1:B:230:PHE:HB3	1.81	0.62
1:F:249:PRO:HD2	1:F:348:GLN:HE21	1.64	0.62
1:B:53:MET:CE	1:B:230:PHE:HB3	2.30	0.62
1:D:139:ILE:HG21	1:D:204:MET:HG2	1.82	0.61
1:E:139:ILE:HG21	1:E:204:MET:HG2	1.83	0.60
1:B:139:ILE:HG21	1:B:204:MET:HG2	1.84	0.60
1:C:281:VAL:HG12	1:C:294:ALA:HB2	1.84	0.60
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.82	0.59
1:C:139:ILE:HG21	1:C:204:MET:HG2	1.84	0.59
1:F:20:PRO:O	1:F:48:ASP:HB3	2.03	0.58
1:F:70:VAL:HG11	1:F:97:MET:SD	2.44	0.58
1:E:247:VAL:HG13	2:K:73:LEU:HD22	1.86	0.58
1:D:128:PHE:HA	1:D:186:GLN:HE22	1.71	0.56
1:F:68:THR:HG21	1:F:92:LEU:HD21	1.87	0.56
1:A:139:ILE:HG21	1:A:204:MET:HG2	1.87	0.56
1:F:6:GLU:OE2	1:F:8:GLU:HG2	2.06	0.55
1:F:338:MET:HE3	1:F:347:VAL:HG21	1.89	0.55
1:D:65:PRO:HD2	1:F:187:SER:O	2.07	0.55
1:E:340:LEU:HG	1:E:347:VAL:HG23	1.89	0.55
1:C:20:PRO:HG2	1:C:53:MET:HG2	1.90	0.54
1:E:1:MET:CE	1:E:37:VAL:HG23	2.38	0.54
1:A:284:TYR:CE1	1:A:316:GLU:HG3	2.43	0.54
1:F:247:VAL:HG13	2:L:73:LEU:HD22	1.90	0.54
1:B:170:VAL:HG22	1:B:179:VAL:HG23	1.89	0.54
1:A:32:ASN:HB3	1:A:69:THR:CG2	2.20	0.53
1:C:128:PHE:HB3	1:C:188:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:MET:HG2	1:E:349:ILE:HG12	1.91	0.53
1:E:39:ASP:CG	1:E:39:ASP:O	2.47	0.53
1:E:1:MET:HE1	1:E:35:LEU:HB3	1.91	0.53
1:D:249:PRO:HB2	1:D:252:PRO:HG3	1.91	0.52
1:D:284:TYR:CE1	1:D:316:GLU:HG3	2.44	0.52
1:D:340:LEU:HG	1:D:347:VAL:HG23	1.89	0.52
1:F:340:LEU:HG	1:F:347:VAL:HG23	1.91	0.52
1:A:340:LEU:HG	1:A:347:VAL:HG23	1.91	0.51
1:B:150:ASP:OD2	1:B:152:ARG:HD3	2.11	0.51
1:A:2:LYS:HB3	1:A:64:GLU:HB3	1.93	0.51
1:E:249:PRO:HB2	1:E:252:PRO:HG3	1.93	0.51
1:D:39:ASP:OD2	1:D:39:ASP:CB	2.58	0.51
1:B:249:PRO:HB2	1:B:252:PRO:HG3	1.92	0.51
1:C:340:LEU:HG	1:C:347:VAL:HG23	1.93	0.51
1:E:170:VAL:HG22	1:E:179:VAL:HG23	1.92	0.51
1:B:340:LEU:HG	1:B:347:VAL:HG23	1.92	0.51
1:C:2:LYS:HB3	1:C:64:GLU:HB3	1.92	0.50
1:A:170:VAL:HG22	1:A:179:VAL:HG23	1.92	0.50
1:C:6:GLU:HB3	1:C:9:HIS:HD2	1.76	0.50
1:D:52:GLU:HG2	1:D:119:LEU:HD22	1.93	0.50
1:B:144:PHE:CD2	1:B:326:ASP:HB3	2.47	0.50
1:D:280:GLY:CA	1:D:364:MET:CE	2.82	0.50
1:B:13:PRO:HA	1:B:230:PHE:HE1	1.76	0.50
1:D:13:PRO:HA	1:D:230:PHE:HE1	1.77	0.50
1:E:360:VAL:HG12	2:K:73:LEU:HD21	1.94	0.50
1:F:338:MET:HG2	1:F:349:ILE:HG12	1.94	0.50
1:D:338:MET:HG2	1:D:349:ILE:HG12	1.93	0.50
1:D:33:LEU:HG	1:D:72:ALA:HB2	1.94	0.50
1:B:2:LYS:HB3	1:B:64:GLU:HB3	1.94	0.49
1:F:184:ILE:HD11	1:F:188:LEU:HD11	1.95	0.49
1:E:13:PRO:HA	1:E:230:PHE:HE1	1.77	0.49
1:D:100:ARG:HG2	1:D:105:ARG:HG3	1.94	0.49
1:E:2:LYS:HB3	1:E:64:GLU:HB2	1.94	0.49
1:D:338:MET:HE3	1:D:347:VAL:HG21	1.95	0.49
1:E:150:ASP:OD2	1:E:152:ARG:HD3	2.12	0.49
1:A:150:ASP:OD1	1:A:152:ARG:HD3	2.12	0.49
1:A:144:PHE:CD2	1:A:326:ASP:HB3	2.48	0.48
1:C:338:MET:HE3	1:C:347:VAL:HG21	1.95	0.48
1:D:70:VAL:HG11	1:D:97:MET:SD	2.53	0.48
1:C:255:HIS:HD2	1:C:339:MET:HG2	1.78	0.48
1:B:247:VAL:HG13	2:H:73:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:MET:HE3	1:B:347:VAL:HG21	1.96	0.48
1:C:170:VAL:HG22	1:C:179:VAL:HG23	1.96	0.48
1:A:53:MET:HB3	1:A:230:PHE:CZ	2.49	0.48
1:F:156:ASN:O	1:F:197:ARG:HB2	2.14	0.48
1:D:257:GLU:HG2	1:D:337:ARG:HG2	1.96	0.48
1:A:127:GLU:CD	1:C:39:ASP:H	2.17	0.47
1:D:170:VAL:HG22	1:D:179:VAL:HG23	1.95	0.47
1:F:150:ASP:OD2	1:F:152:ARG:HD3	2.15	0.47
1:C:144:PHE:CD2	1:C:326:ASP:HB3	2.49	0.47
1:A:21:LEU:H	1:A:21:LEU:HD12	1.80	0.47
1:A:338:MET:HE3	1:A:347:VAL:HG21	1.97	0.47
1:F:147:ALA:HB2	1:F:173:ASP:HA	1.97	0.47
1:F:33:LEU:HG	1:F:72:ALA:HB2	1.96	0.47
1:C:70:VAL:HG11	1:C:97:MET:SD	2.55	0.47
1:F:170:VAL:HG22	1:F:179:VAL:HG23	1.98	0.46
1:B:360:VAL:HG12	2:H:73:LEU:HD21	1.96	0.46
1:C:17:VAL:HG23	1:C:33:LEU:HD11	1.97	0.46
1:A:127:GLU:HG3	1:A:217:GLN:HG2	1.98	0.46
1:D:247:VAL:HG13	2:J:73:LEU:HD22	1.98	0.46
1:F:2:LYS:HD2	1:F:91:GLN:HB2	1.97	0.46
1:A:146:MET:HE1	1:A:197:ARG:HA	1.98	0.46
1:D:146:MET:HE1	1:D:197:ARG:HA	1.98	0.46
1:A:338:MET:HG2	1:A:349:ILE:HG12	1.97	0.46
1:B:33:LEU:HG	1:B:72:ALA:HB2	1.98	0.46
1:D:144:PHE:CD2	1:D:326:ASP:HB3	2.50	0.46
1:A:147:ALA:HB1	1:A:150:ASP:HB2	1.98	0.46
1:E:155:LEU:HD22	1:E:172:THR:HG23	1.97	0.45
1:E:33:LEU:HG	1:E:72:ALA:HB2	1.98	0.45
1:C:20:PRO:HG3	1:C:202:GLU:OE1	2.16	0.45
1:D:281:VAL:HG12	1:D:294:ALA:HB2	1.98	0.45
1:D:17:VAL:HG12	1:D:53:MET:HG3	1.97	0.45
1:F:33:LEU:O	1:F:69:THR:HA	2.16	0.45
1:E:144:PHE:CD2	1:E:326:ASP:HB3	2.51	0.45
1:A:50:GLU:HA	1:A:235:LYS:HD2	1.99	0.44
1:B:147:ALA:O	1:B:197:ARG:NH1	2.46	0.44
1:C:206:MET:HE2	1:C:227:VAL:HG12	1.99	0.44
1:C:150:ASP:OD2	1:C:152:ARG:HD3	2.18	0.44
1:D:249:PRO:HD2	1:D:348:GLN:NE2	2.32	0.44
1:E:147:ALA:HB2	1:E:173:ASP:HA	1.98	0.44
1:E:174:GLY:HA2	2:K:74:PHE:CZ	2.52	0.44
1:C:155:LEU:HD22	1:C:172:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ALA:HB2	1:B:173:ASP:HA	1.98	0.44
1:A:33:LEU:HG	1:A:72:ALA:HB2	2.00	0.44
1:F:174:GLY:HA2	2:L:74:PHE:CZ	2.53	0.43
1:D:2:LYS:HG2	1:D:91:GLN:CB	2.48	0.43
1:A:255[A]:HIS:NE2	1:A:339:MET:HG2	2.33	0.43
1:B:16:GLN:HE21	1:B:53:MET:CE	2.29	0.43
1:D:155:LEU:HD22	1:D:172:THR:HG23	2.01	0.43
1:C:147:ALA:HB2	1:C:173:ASP:HA	2.00	0.43
1:E:147:ALA:HB1	1:E:150:ASP:HB2	2.01	0.43
1:E:70:VAL:HG11	1:E:97:MET:SD	2.58	0.43
1:A:263:LEU:HD23	1:A:336:VAL:HG21	1.99	0.43
1:F:346:SER:HA	1:F:363:PRO:HD3	2.01	0.43
1:B:147:ALA:HB1	1:B:150:ASP:HB2	2.00	0.43
1:B:70:VAL:HG11	1:B:97:MET:SD	2.58	0.43
1:D:27:LEU:HB2	1:D:30:LEU:HG	2.01	0.43
1:F:144:PHE:CD2	1:F:326:ASP:HB3	2.54	0.43
1:A:331:LEU:HD13	1:A:336:VAL:HG12	2.00	0.42
1:B:27:LEU:HB2	1:B:30:LEU:HG	2.01	0.42
1:B:338:MET:HG2	1:B:349:ILE:HG12	2.01	0.42
1:D:161:GLU:OE1	1:D:168:ARG:NH2	2.53	0.42
1:D:33:LEU:O	1:D:69:THR:HA	2.19	0.42
1:D:337:ARG:HG3	1:D:352:ALA:HA	2.02	0.42
1:A:346:SER:HA	1:A:363:PRO:HD3	2.02	0.42
1:A:14:LEU:O	1:A:18:SER:HB3	2.20	0.42
1:C:27:LEU:HB2	1:C:30:LEU:HG	2.01	0.41
1:B:15:GLN:HG3	1:B:76:PHE:CE1	2.55	0.41
1:C:12:LYS:HB3	1:C:13:PRO:HD3	2.01	0.41
1:A:159:LEU:O	1:A:169:THR:HA	2.21	0.41
1:A:27:LEU:HB2	1:A:30:LEU:HG	2.01	0.41
1:D:217:GLN:NE2	1:D:226:HIS:NE2	2.68	0.41
1:D:156:ASN:O	1:D:197:ARG:HB2	2.21	0.41
1:A:295:ASN:HA	1:A:300:GLU:O	2.21	0.41
1:D:285:VAL:HG12	1:D:290:LEU:HD13	2.03	0.41
1:A:283:LEU:O	1:A:316:GLU:HA	2.21	0.41
1:F:27:LEU:HB2	1:F:30:LEU:HG	2.03	0.41
1:E:159:LEU:O	1:E:169:THR:HA	2.22	0.40
1:F:339:MET:CE	1:F:350:GLU:HG2	2.51	0.40
1:E:249:PRO:HD2	1:E:348:GLN:NE2	2.30	0.40
1:A:156:ASN:O	1:A:197:ARG:HB2	2.21	0.40
1:D:128:PHE:HB3	1:D:188:LEU:HD21	2.04	0.40
1:B:50:GLU:HA	1:B:235:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:ASN:HA	1:F:300:GLU:O	2.22	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	365/366 (100%)	353 (97%)	11 (3%)	1 (0%)	46	57
1	B	360/366 (98%)	350 (97%)	9 (2%)	1 (0%)	46	57
1	C	363/366 (99%)	351 (97%)	12 (3%)	0	100	100
1	D	363/366 (99%)	355 (98%)	8 (2%)	0	100	100
1	E	360/366 (98%)	351 (98%)	8 (2%)	1 (0%)	46	57
1	F	363/366 (99%)	356 (98%)	7 (2%)	0	100	100
2	H	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
2	I	4/6 (67%)	4 (100%)	0	0	100	100
2	J	4/6 (67%)	4 (100%)	0	0	100	100
2	K	4/6 (67%)	4 (100%)	0	0	100	100
2	L	4/6 (67%)	4 (100%)	0	0	100	100
All	All	2194/2226 (99%)	2135 (97%)	56 (3%)	3 (0%)	56	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	39	ASP
1	B	49	LEU
1	A	22	GLY



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/313 (95%)	291 (98%)	5 (2%)	68	83
1	B	303/313 (97%)	292 (96%)	11 (4%)	42	57
1	C	297/313 (95%)	287 (97%)	10 (3%)	44	59
1	D	297/313 (95%)	288 (97%)	9 (3%)	48	65
1	E	297/313 (95%)	291 (98%)	6 (2%)	63	79
1	F	303/313 (97%)	294 (97%)	9 (3%)	48	65
2	H	5/5 (100%)	4 (80%)	1 (20%)	1	1
2	I	5/5 (100%)	4 (80%)	1 (20%)	1	1
2	J	5/5 (100%)	4 (80%)	1 (20%)	1	1
2	K	5/5 (100%)	5 (100%)	0	100	100
2	L	5/5 (100%)	4 (80%)	1 (20%)	1	1
All	All	1818/1903 (96%)	1764 (97%)	54 (3%)	48	65

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	176	ARG
1	A	188	LEU
1	A	192	SER
1	A	212	ASN
1	B	26	THR
1	B	39	ASP
1	B	56	ARG
1	B	125	GLU
1	B	129	THR
1	B	176	ARG
1	B	184	ILE
1	B	191	HIS
1	B	212	ASN
1	B	253	ASP

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Mol	Chain	Res	Type
1	B	295	ASN
1	C	21	LEU
1	C	39	ASP
1	C	87	GLU
1	C	129	THR
1	C	176	ARG
1	C	192	SER
1	C	212	ASN
1	C	253	ASP
1	C	285	VAL
1	C	355	GLN
1	D	56	ARG
1	D	93	GLU
1	D	121	ASP
1	D	123	GLN
1	D	129	THR
1	D	176	ARG
1	D	253	ASP
1	D	334	GLU
1	D	364	MET
1	E	64	GLU
1	E	129	THR
1	E	176	ARG
1	E	192	SER
1	E	334	GLU
1	E	355	GLN
1	F	11	LEU
1	F	27	LEU
1	F	62	PRO
1	F	84	GLU
1	F	129	THR
1	F	176	ARG
1	F	192	SER
1	F	251	ASN
1	F	285	VAL
2	H	72	ASP
2	I	72	ASP
2	J	72	ASP
2	L	72	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	61	GLN
1	A	191	HIS
1	A	217	GLN
1	A	335	ASN
1	A	348	GLN
1	B	16	GLN
1	B	61	GLN
1	B	143	GLN
1	B	217	GLN
1	B	265	GLN
1	B	335	ASN
1	B	348	GLN
1	C	9	HIS
1	C	91	GLN
1	C	191	HIS
1	C	255	HIS
1	C	265	GLN
1	C	335	ASN
1	C	348	GLN
1	D	16	GLN
1	D	186	GLN
1	D	191	HIS
1	D	217	GLN
1	D	265	GLN
1	D	335	ASN
1	D	348	GLN
1	E	191	HIS
1	E	217	GLN
1	E	265	GLN
1	E	335	ASN
1	E	348	GLN
1	F	9	HIS
1	F	191	HIS
1	F	217	GLN
1	F	265	GLN
1	F	335	ASN
1	F	348	GLN
2	I	70	GLN
2	J	70	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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	366/366 (100%)	0.39	20 (5%) 29 37	27, 57, 85, 104	1 (0%)
1	B	364/366 (99%)	0.07	9 (2%) 61 70	23, 45, 72, 97	2 (0%)
1	C	365/366 (99%)	0.32	21 (5%) 26 35	31, 55, 80, 101	2 (0%)
1	D	365/366 (99%)	0.31	15 (4%) 41 50	32, 54, 83, 95	1 (0%)
1	E	364/366 (99%)	0.17	15 (4%) 41 50	26, 51, 76, 107	1 (0%)
1	F	365/366 (99%)	0.03	10 (2%) 58 67	29, 47, 75, 99	1 (0%)
2	H	5/6 (83%)	0.44	0 100 100	44, 45, 58, 59	0
2	I	5/6 (83%)	2.17	3 (60%) 0 0	62, 67, 74, 78	0
2	J	5/6 (83%)	3.25	3 (60%) 0 0	78, 90, 100, 108	0
2	K	5/6 (83%)	1.07	0 100 100	54, 54, 65, 66	0
2	L	5/6 (83%)	1.99	3 (60%) 0 0	66, 72, 81, 86	0
All	All	2214/2226 (99%)	0.23	99 (4%) 37 46	23, 52, 81, 108	8 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	23	GLY	7.8
1	D	23	GLY	7.3
1	A	22	GLY	6.8
1	A	366	LEU	6.3
2	J	74	PHE	5.8
1	C	22	GLY	5.4
1	A	23	GLY	5.4
1	A	21	LEU	5.3
1	A	153	TYR	5.2
1	C	60	VAL	5.0
1	D	24	ARG	5.0
1	B	20	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	211	ASP	4.4
1	F	26	THR	4.3
1	A	187	SER	4.2
1	D	22	GLY	4.1
1	E	24	ARG	4.1
2	J	71	LEU	4.1
2	I	71	LEU	4.0
2	L	74	PHE	3.9
1	E	94	GLY	3.9
1	A	20	PRO	3.7
2	J	72	ASP	3.6
1	E	121	ASP	3.5
1	E	211	ASP	3.5
1	C	40	GLY	3.5
1	B	26	THR	3.5
2	I	74	PHE	3.4
1	E	208	ASP	3.4
1	D	315	MET	3.3
1	E	210	GLY	3.3
1	C	114	ALA	3.2
1	E	153	TYR	3.2
1	A	311	SER	3.2
1	F	23	GLY	3.2
1	B	24	ARG	3.1
1	C	255	HIS	3.1
2	L	72	ASP	3.0
1	A	133	ALA	3.0
1	D	208	ASP	2.9
1	A	148	HIS	2.9
1	A	246	ARG	2.9
1	F	22	GLY	2.8
1	C	58	ALA	2.8
1	C	85	GLY	2.8
1	D	209	GLY	2.8
1	E	114	ALA	2.8
1	E	209	GLY	2.7
1	D	120	ASP	2.7
1	B	187	SER	2.7
1	F	299	GLN	2.7
1	F	118	ASN	2.7
1	E	21	LEU	2.6
1	B	60	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	311	SER	2.6
1	F	24	ARG	2.6
1	A	120	ASP	2.6
1	B	238	ASP	2.6
1	C	308	VAL	2.6
1	C	117	PRO	2.5
1	F	149	GLN	2.5
1	A	209	GLY	2.5
1	A	26	THR	2.5
1	C	119	LEU	2.5
1	A	149	GLN	2.4
1	C	120	ASP	2.4
1	D	25	PRO	2.4
1	A	60	VAL	2.4
1	B	84	GLU	2.4
1	C	151	VAL	2.4
1	C	26	THR	2.4
1	C	313	ALA	2.4
2	L	71	LEU	2.4
1	C	62	PRO	2.4
1	C	35	LEU	2.3
1	D	362	MET	2.3
1	E	26	THR	2.3
1	E	187	SER	2.3
1	F	250	LYS	2.2
1	A	191	HIS	2.2
1	C	55	ALA	2.2
1	D	148	HIS	2.2
1	A	365	ARG	2.2
1	E	39	ASP	2.1
1	D	151	VAL	2.1
1	D	247	VAL	2.1
1	B	25	PRO	2.1
1	C	353	ALA	2.1
1	E	18	SER	2.1
2	I	72	ASP	2.1
1	A	24	ARG	2.1
1	F	309	THR	2.1
1	B	94	GLY	2.1
1	F	251	ASN	2.0
1	A	208	ASP	2.0
1	C	84	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	313	ALA	2.0
1	E	311	SER	2.0
1	D	244	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.