



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:42 PM GMT

PDB ID : 1LMK  
Title : THE STRUCTURE OF A BIVALENT DIABODY  
Authors : Williams, R.L.  
Deposited on : 1994-08-29  
Resolution : 2.60 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

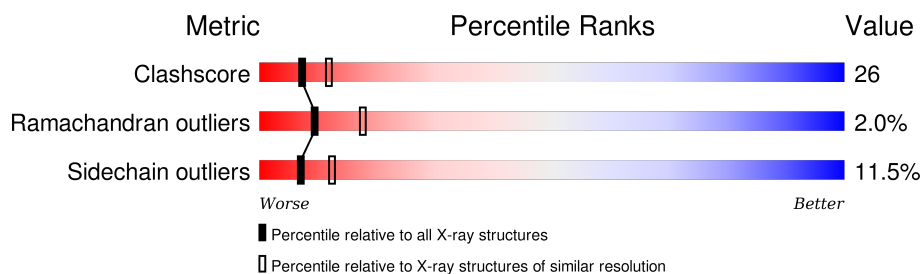
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	238	 58% 34% 8%
1	C	238	 57% 36% 7%
1	E	238	 47% 45% 8%
1	G	238	 49% 42% 9%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7613 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 ANTI-PHOSPHATIDYLINOSITOL SPECIFIC PHOSPHOLIPASE C DIABODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	61	0	0
			1838	1167	305	360	6			
1	C	238	Total	C	N	O	S	30	0	0
			1838	1167	305	360	6			
1	E	238	Total	C	N	O	S	64	0	0
			1838	1167	305	360	6			
1	G	238	Total	C	N	O	S	37	0	0
			1838	1167	305	360	6			

- Molecule 2 is water.

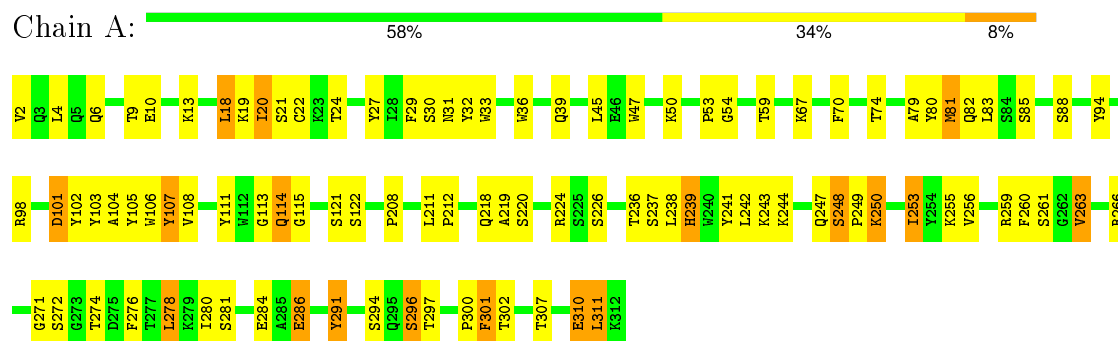
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total	O	0	0
			72	72		
2	C	65	Total	O	0	0
			65	65		
2	E	66	Total	O	0	0
			66	66		
2	G	58	Total	O	0	0
			58	58		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

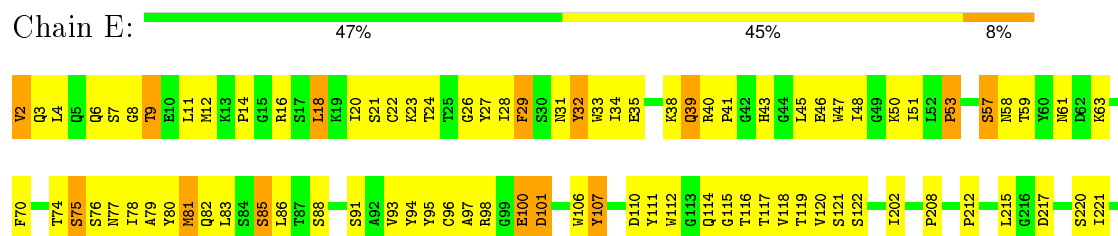
#### • Molecule 1: ANTI-PHOSPHATIDYLINOSITOL SPECIFIC PHOSPHOLIPASE C DIABODY

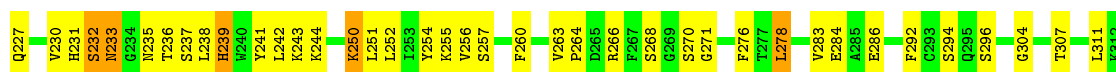


#### • Molecule 1: ANTI-PHOSPHATIDYLINOSITOL SPECIFIC PHOSPHOLIPASE C DIABODY

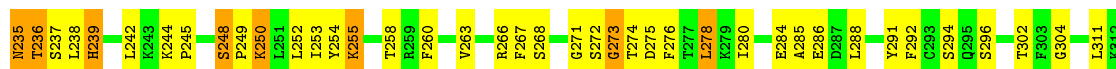
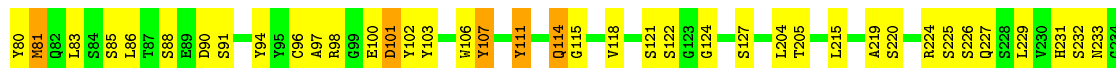


#### • Molecule 1: ANTI-PHOSPHATIDYLINOSITOL SPECIFIC PHOSPHOLIPASE C DIABODY





- Molecule 1: ANTI-PHOSPHATIDYLINOSITOL SPECIFIC PHOSPHOLIPASE C DIA-BODY



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.14Å 80.71Å 88.01Å 90.00° 99.81° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7613	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

## 5 Model quality [i](#)

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

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	0.89	0/1885	1.04	1/2554 (0.0%)
1	C	0.93	0/1885	1.04	1/2554 (0.0%)
1	E	0.91	0/1885	1.06	4/2554 (0.2%)
1	G	0.83	0/1885	1.01	0/2554
All	All	0.89	0/7540	1.03	6/10216 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	G	0	2
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	238	LEU	CA-CB-CG	-6.42	100.53	115.30
1	A	238	LEU	CA-CB-CG	-5.83	101.89	115.30
1	E	101	ASP	CB-CG-OD1	5.74	123.47	118.30
1	E	38	LYS	CD-CE-NZ	-5.42	99.23	111.70
1	C	253	ILE	CG1-CB-CG2	-5.30	99.74	111.40
1	E	230	VAL	CB-CA-C	-5.14	101.64	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	TYR	Sidechain
1	C	291	TYR	Sidechain
1	E	32	TYR	Sidechain
1	G	103	TYR	Sidechain
1	G	111	TYR	Sidechain

## 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	1838	0	1777	87	0
1	C	1838	0	1777	92	0
1	E	1838	0	1777	100	0
1	G	1838	0	1777	99	0
2	A	72	0	0	4	0
2	C	65	0	0	4	0
2	E	66	0	0	3	0
2	G	58	0	0	5	0
All	All	7613	0	7108	364	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 26.

All (364) 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:C:39:GLN:HG3	1:C:45:LEU:HD23	1.41	1.01
1:A:39:GLN:HG2	1:A:45:LEU:HD23	1.47	0.95
1:C:20:ILE:HG21	1:C:116:THR:HG21	1.50	0.93
1:E:2:VAL:HG11	1:E:98:ARG:HH21	1.35	0.91
1:A:114:GLN:H	1:A:114:GLN:HE21	1.19	0.90
1:E:39:GLN:HG2	1:E:45:LEU:HD23	1.56	0.88
1:G:114:GLN:H	1:G:114:GLN:HE21	1.19	0.88
1:C:114:GLN:H	1:C:114:GLN:HE21	1.22	0.88
1:C:244:LYS:HD3	1:C:250:LYS:HE2	1.53	0.87
1:E:23:LYS:HG3	1:E:78:ILE:HG12	1.57	0.87
1:E:244:LYS:HD3	1:E:250:LYS:HE2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:SER:HB3	1:G:122:SER:OG	1.80	0.81
1:A:114:GLN:N	1:A:114:GLN:HE21	1.79	0.81
1:A:2:VAL:HG11	1:A:98:ARG:NH2	1.96	0.80
1:A:39:GLN:CG	1:A:45:LEU:HD23	2.12	0.79
1:A:2:VAL:HG11	1:A:98:ARG:HH21	1.47	0.79
1:C:10:GLU:HG3	1:C:18:LEU:HD12	1.65	0.77
1:G:51:ILE:HG13	1:G:58:ASN:OD1	1.82	0.76
1:E:18:LEU:HD22	1:E:86:LEU:HD11	1.67	0.76
1:A:211:LEU:HD21	1:A:219:ALA:HB1	1.69	0.75
1:G:233:ASN:HB2	1:G:235:ASN:OD1	1.86	0.74
1:A:4:LEU:CD2	1:A:24:THR:HG22	2.18	0.74
1:A:70:PHE:HE1	1:A:81:MET:HG3	1.53	0.72
1:A:18:LEU:CD2	1:A:83:LEU:HD12	2.20	0.72
1:E:11:LEU:HD12	1:E:119:THR:O	1.90	0.72
1:G:70:PHE:CE1	1:G:81:MET:HG3	2.25	0.71
1:C:237:SER:O	1:C:295:GLN:HA	1.91	0.71
1:C:114:GLN:N	1:C:114:GLN:HE21	1.89	0.71
1:G:271:GLY:HA3	1:G:276:PHE:HA	1.70	0.71
1:C:10:GLU:HG3	1:C:18:LEU:CD1	2.20	0.70
1:A:237:SER:HB2	1:A:297:THR:OG1	1.90	0.70
1:G:101:ASP:HB3	1:G:106:TRP:HB3	1.71	0.70
1:C:233:ASN:C	1:C:233:ASN:HD22	1.92	0.69
1:A:70:PHE:CE1	1:A:81:MET:HG3	2.28	0.69
1:G:2:VAL:HG11	1:G:98:ARG:NH2	2.08	0.68
1:C:39:GLN:CG	1:C:45:LEU:HD23	2.18	0.68
1:G:3:GLN:O	1:G:4:LEU:HD23	1.93	0.68
1:C:233:ASN:ND2	1:C:235:ASN:H	1.91	0.68
1:C:100:GLU:HG2	1:C:101:ASP:N	2.08	0.68
1:C:39:GLN:HG3	1:C:45:LEU:CD2	2.21	0.68
1:C:215:LEU:HG	1:C:311:LEU:HD11	1.77	0.67
1:C:114:GLN:NE2	1:C:114:GLN:H	1.92	0.67
1:E:239:HIS:HD2	1:E:255:LYS:H	1.41	0.67
1:G:114:GLN:N	1:G:114:GLN:HE21	1.91	0.67
1:G:70:PHE:HE1	1:G:81:MET:HG3	1.60	0.67
1:C:233:ASN:HD22	1:C:234:GLY:N	1.91	0.67
1:G:219:ALA:HA	2:G:350:HOH:O	1.93	0.66
1:G:266:ARG:CZ	1:G:284:GLU:HG3	2.26	0.66
1:G:28:ILE:O	1:G:31:ASN:HB2	1.96	0.66
1:E:51:ILE:O	1:E:53:PRO:HD3	1.96	0.65
1:A:32:TYR:CG	1:A:98:ARG:HD3	2.32	0.65
1:E:2:VAL:HG11	1:E:98:ARG:NH2	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:LYS:H	1:G:250:LYS:HZ1	1.44	0.64
1:G:6:GLN:HA	1:G:21:SER:O	1.97	0.64
1:A:244:LYS:HD3	1:A:250:LYS:HE2	1.78	0.64
1:A:249:PRO:HD2	1:C:112:TRP:CE3	2.33	0.64
1:E:233:ASN:HD22	1:E:235:ASN:H	1.46	0.64
1:E:215:LEU:HG	1:E:311:LEU:HD11	1.80	0.64
1:E:266:ARG:CZ	1:E:284:GLU:HG3	2.27	0.64
1:G:6:GLN:H	1:G:114:GLN:HE22	1.46	0.63
1:C:2:VAL:N	2:C:324:HOH:O	2.31	0.63
1:A:6:GLN:H	1:A:114:GLN:HE22	1.46	0.63
1:E:202:ILE:HD11	1:E:227:GLN:OE1	1.98	0.63
1:C:211:LEU:HD21	1:C:219:ALA:HB1	1.80	0.63
1:G:292:PHE:CD1	1:G:304:GLY:O	2.52	0.63
1:G:91:SER:HA	1:G:118:VAL:O	1.99	0.63
1:G:231:HIS:ND1	1:G:233:ASN:OD1	2.32	0.63
1:A:114:GLN:H	1:A:114:GLN:NE2	1.95	0.62
1:E:14:PRO:HG2	1:E:122:SER:HB3	1.80	0.62
1:G:39:GLN:HG2	1:G:45:LEU:HD23	1.83	0.61
1:G:18:LEU:CD2	1:G:83:LEU:HD12	2.30	0.61
1:G:242:LEU:O	1:G:250:LYS:NZ	2.34	0.61
1:G:260:PHE:O	1:G:263:VAL:HG23	2.00	0.60
1:C:253:ILE:HG21	1:C:256:VAL:O	2.01	0.60
1:C:70:PHE:CE1	1:C:81:MET:HG3	2.36	0.60
1:A:94:TYR:O	1:A:115:GLY:HA2	2.02	0.60
1:E:217:ASP:O	1:E:283:VAL:HG23	2.01	0.60
1:G:292:PHE:HD1	1:G:304:GLY:O	1.85	0.60
1:G:94:TYR:O	1:G:115:GLY:HA2	2.01	0.60
1:E:23:LYS:CG	1:E:78:ILE:HG12	2.30	0.60
1:A:272:SER:HA	2:A:357:HOH:O	2.02	0.60
1:A:27:TYR:CE2	1:A:32:TYR:HD2	2.20	0.59
1:E:251:LEU:HD23	1:E:260:PHE:CD1	2.36	0.59
1:G:215:LEU:HG	1:G:311:LEU:HD11	1.83	0.59
1:A:4:LEU:HD22	1:A:24:THR:HG22	1.84	0.59
1:G:32:TYR:CG	1:G:98:ARG:HD3	2.38	0.59
1:A:260:PHE:O	1:A:263:VAL:HG13	2.02	0.59
1:E:12:MET:HG3	1:E:86:LEU:CD1	2.33	0.59
1:A:22:CYS:HB3	1:A:79:ALA:HB3	1.84	0.59
1:E:33:TRP:CE3	1:E:50:LYS:HE3	2.37	0.59
1:G:254:TYR:HD2	1:G:255:LYS:HD3	1.67	0.59
1:E:252:LEU:HA	1:E:263:VAL:HG21	1.84	0.58
1:A:208:PRO:O	1:A:307:THR:HG23	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:ASN:HD22	1:E:233:ASN:C	2.05	0.58
1:E:3:GLN:C	1:E:4:LEU:HD12	2.22	0.58
1:C:54:GLY:O	1:C:56:GLY:N	2.37	0.58
1:G:29:PHE:CE2	1:G:53:PRO:HB3	2.37	0.58
1:C:239:HIS:HD2	1:C:255:LYS:H	1.52	0.57
1:E:235:ASN:HD22	1:E:255:LYS:HD2	1.68	0.57
1:E:32:TYR:CG	1:E:98:ARG:HD3	2.38	0.57
1:A:239:HIS:HE1	1:A:296:SER:OG	1.87	0.57
1:G:29:PHE:CE2	1:G:53:PRO:CB	2.88	0.57
1:E:239:HIS:CD2	1:E:255:LYS:H	2.23	0.56
1:C:2:VAL:HG11	1:C:98:ARG:NH2	2.20	0.56
1:C:239:HIS:CD2	1:C:255:LYS:H	2.23	0.56
1:C:251:LEU:HD23	1:C:260:PHE:CD1	2.41	0.56
1:C:100:GLU:HG2	1:C:101:ASP:H	1.70	0.56
1:C:20:ILE:CG2	1:C:116:THR:HG21	2.32	0.56
1:E:241:TYR:HE1	1:E:294:SER:HG	1.54	0.56
1:E:46:GLU:HG2	2:E:334:HOH:O	2.04	0.56
1:A:224:ARG:HA	1:A:274:THR:O	2.05	0.56
1:G:72:ALA:HA	1:G:79:ALA:HA	1.88	0.56
1:A:21:SER:HB3	1:A:80:TYR:CE1	2.41	0.56
1:G:244:LYS:HD3	1:G:250:LYS:HE2	1.85	0.56
1:A:36:TRP:CE3	1:A:81:MET:HE2	2.41	0.55
1:A:255:LYS:NZ	1:C:108:VAL:HG23	2.21	0.55
1:A:27:TYR:CD2	1:A:32:TYR:CD2	2.95	0.55
1:A:31:ASN:O	1:A:102:TYR:N	2.36	0.55
1:E:50:LYS:HG2	1:E:59:THR:HB	1.88	0.55
1:G:244:LYS:HB2	1:G:250:LYS:HE2	1.87	0.55
1:G:47:TRP:HZ2	1:G:50:LYS:HD2	1.71	0.55
1:E:254:TYR:HD2	1:E:255:LYS:HG3	1.72	0.55
1:G:3:GLN:C	1:G:4:LEU:HD23	2.27	0.54
1:E:70:PHE:CE1	1:E:81:MET:HG3	2.42	0.54
1:E:95:TYR:CE1	1:G:248:SER:HB3	2.42	0.54
1:E:100:GLU:HA	1:E:107:TYR:HA	1.89	0.54
1:A:27:TYR:CD2	1:A:32:TYR:HD2	2.25	0.54
1:G:231:HIS:ND1	1:G:232:SER:N	2.55	0.54
1:G:10:GLU:HG3	1:G:18:LEU:HD11	1.89	0.54
1:C:13:LYS:O	1:C:16:ARG:HB2	2.08	0.54
1:E:33:TRP:CH2	1:E:57:SER:HB3	2.43	0.54
1:E:27:TYR:OH	1:E:34:ILE:HD11	2.07	0.54
1:A:2:VAL:N	2:A:353:HOH:O	2.41	0.53
1:C:233:ASN:C	1:C:233:ASN:ND2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:ARG:HA	1:G:274:THR:O	2.07	0.53
1:E:63:LYS:HE2	2:E:338:HOH:O	2.08	0.53
1:C:2:VAL:HG11	1:C:98:ARG:HH21	1.73	0.53
1:A:10:GLU:HG3	1:A:18:LEU:CD1	2.38	0.53
1:A:107:TYR:CG	1:C:296:SER:HB3	2.43	0.53
1:E:14:PRO:CG	1:E:122:SER:HB3	2.39	0.53
1:C:271:GLY:HA3	1:C:276:PHE:HA	1.89	0.53
1:G:253:ILE:HA	1:G:258:THR:O	2.09	0.53
1:A:266:ARG:CZ	1:A:284:GLU:HG3	2.39	0.52
1:A:107:TYR:CD2	1:C:296:SER:HB3	2.44	0.52
1:G:32:TYR:CD1	1:G:101:ASP:HA	2.44	0.52
1:G:254:TYR:O	1:G:255:LYS:C	2.47	0.52
1:A:101:ASP:OD2	1:A:103:TYR:N	2.43	0.52
1:E:76:SER:O	1:E:77:ASN:HB2	2.09	0.52
1:C:6:GLN:H	1:C:114:GLN:HE22	1.57	0.51
1:E:244:LYS:H	1:E:250:LYS:HZ1	1.58	0.51
1:A:2:VAL:HG22	1:A:111:TYR:CG	2.44	0.51
1:E:18:LEU:O	1:E:82:GLN:HG3	2.09	0.51
1:G:97:ALA:HA	1:G:111:TYR:O	2.10	0.51
1:E:22:CYS:N	1:E:79:ALA:O	2.43	0.51
1:E:237:SER:HB3	2:G:338:HOH:O	2.09	0.51
1:E:296:SER:HB2	2:G:338:HOH:O	2.09	0.51
1:C:3:GLN:HB2	1:C:25:THR:OG1	2.10	0.51
1:E:237:SER:HB3	1:E:296:SER:HB2	1.91	0.51
1:A:106:TRP:CZ2	1:A:108:VAL:HB	2.45	0.51
1:C:29:PHE:CE2	1:C:53:PRO:HB3	2.46	0.51
1:C:38:LYS:HB2	1:C:48:ILE:HD11	1.92	0.51
1:G:2:VAL:HG11	1:G:98:ARG:HH21	1.74	0.51
1:E:88:SER:HB3	1:E:122:SER:OG	2.11	0.51
1:E:110:ASP:HB2	1:G:260:PHE:CZ	2.45	0.51
1:A:88:SER:HB3	1:A:122:SER:OG	2.10	0.51
1:A:239:HIS:CE1	1:A:296:SER:OG	2.64	0.51
1:A:255:LYS:HZ1	1:C:108:VAL:HG23	1.76	0.51
1:G:3:GLN:HB2	1:G:25:THR:HG22	1.93	0.50
1:E:233:ASN:ND2	1:E:235:ASN:H	2.07	0.50
1:G:224:ARG:NH1	2:G:347:HOH:O	2.45	0.50
1:G:102:TYR:C	1:G:102:TYR:CD1	2.84	0.50
1:E:221:ILE:HG23	1:E:307:THR:HG21	1.93	0.50
1:A:296:SER:HB3	1:C:107:TYR:CD2	2.47	0.50
1:C:22:CYS:N	1:C:79:ALA:O	2.44	0.50
1:C:39:GLN:HG2	1:C:44:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:ASP:HB3	1:G:76:SER:OG	2.11	0.50
1:C:9:THR:HB	1:C:117:THR:HB	1.92	0.50
1:G:67:LYS:NZ	1:G:90:ASP:OD2	2.44	0.50
1:G:252:LEU:HD11	1:G:291:TYR:CE2	2.46	0.49
1:C:88:SER:HB3	1:C:122:SER:OG	2.12	0.49
1:C:20:ILE:O	1:C:80:TYR:HA	2.13	0.49
1:C:51:ILE:O	1:C:53:PRO:HD3	2.13	0.49
1:A:54:GLY:HA2	1:A:74:THR:HG21	1.94	0.49
1:A:284:GLU:HB2	1:A:286:GLU:HG3	1.94	0.49
1:G:29:PHE:HE2	1:G:53:PRO:HB3	1.78	0.49
1:G:229:LEU:O	1:G:236:THR:HA	2.12	0.49
1:A:236:THR:O	1:A:255:LYS:HA	2.13	0.49
1:G:60:TYR:CE1	1:G:70:PHE:CE2	3.01	0.48
1:C:29:PHE:HB3	2:C:320:HOH:O	2.13	0.48
1:G:273:GLY:O	1:G:276:PHE:CZ	2.67	0.48
1:A:311:LEU:HD23	1:A:311:LEU:C	2.34	0.48
1:E:40:ARG:O	1:E:43:HIS:HB2	2.13	0.48
1:G:28:ILE:O	1:G:28:ILE:HG22	2.13	0.48
1:G:205:THR:N	1:G:224:ARG:O	2.47	0.48
1:A:248:SER:HB3	1:C:95:TYR:CE1	2.48	0.48
1:E:107:TYR:CD2	1:G:296:SER:HB3	2.49	0.48
1:A:47:TRP:HZ2	1:A:50:LYS:HD2	1.79	0.48
1:G:102:TYR:CD1	1:G:102:TYR:O	2.67	0.47
1:A:271:GLY:HA3	1:A:276:PHE:CD1	2.49	0.47
1:C:36:TRP:HA	1:C:95:TYR:O	2.13	0.47
1:G:32:TYR:CD2	1:G:98:ARG:HD3	2.50	0.47
1:A:218:GLN:HB2	1:A:281:SER:O	2.14	0.47
1:E:91:SER:HA	1:E:118:VAL:O	2.14	0.47
1:A:212:PRO:HA	1:A:310:GLU:O	2.13	0.47
1:C:16:ARG:HD3	1:C:17:SER:O	2.14	0.47
1:G:25:THR:HG23	1:G:26:GLY:N	2.30	0.47
1:A:266:ARG:O	1:A:280:ILE:HA	2.15	0.47
1:E:112:TRP:CE3	1:G:249:PRO:HD2	2.50	0.47
1:A:243:LYS:NZ	1:A:247:GLN:O	2.32	0.47
1:E:20:ILE:O	1:E:80:TYR:HA	2.15	0.47
1:E:220:SER:HA	1:E:278:LEU:O	2.14	0.47
1:C:286:GLU:HG3	1:C:286:GLU:H	1.35	0.47
1:E:8:GLY:O	1:E:116:THR:HG23	2.15	0.47
1:A:27:TYR:CE2	1:A:32:TYR:CD2	3.01	0.47
1:E:33:TRP:CD2	1:E:50:LYS:HE3	2.49	0.47
1:E:3:GLN:O	1:E:4:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:TRP:CZ3	1:C:50:LYS:HG3	2.50	0.47
1:A:22:CYS:N	1:A:79:ALA:O	2.47	0.46
1:E:74:THR:O	1:E:75:SER:C	2.54	0.46
1:C:231:HIS:ND1	1:C:232:SER:N	2.63	0.46
1:C:29:PHE:HB3	1:C:77:ASN:OD1	2.15	0.46
1:E:12:MET:HG3	1:E:86:LEU:HD13	1.97	0.46
1:C:24:THR:HG1	1:C:29:PHE:HD1	1.57	0.46
1:G:272:SER:N	1:G:275:ASP:O	2.49	0.46
1:G:231:HIS:CE1	1:G:233:ASN:OD1	2.68	0.46
1:G:220:SER:HA	1:G:278:LEU:O	2.16	0.46
1:E:32:TYR:CZ	1:E:98:ARG:NH1	2.83	0.46
1:A:67:LYS:O	1:A:83:LEU:HA	2.15	0.46
1:C:17:SER:HB2	1:C:84:SER:HA	1.98	0.46
1:A:2:VAL:CG2	1:A:111:TYR:CG	2.99	0.46
1:G:239:HIS:HD2	1:G:255:LYS:H	1.64	0.46
1:C:241:TYR:HE1	1:C:294:SER:HG	1.64	0.46
1:E:271:GLY:HA3	1:E:276:PHE:HA	1.97	0.46
1:C:210:SER:OG	1:C:310:GLU:OE2	2.33	0.46
1:G:273:GLY:O	1:G:276:PHE:HZ	1.98	0.46
1:E:106:TRP:CE3	1:G:255:LYS:NZ	2.83	0.46
1:E:29:PHE:CE2	1:E:53:PRO:HB3	2.50	0.46
1:E:9:THR:HB	1:E:117:THR:O	2.14	0.46
1:E:100:GLU:HG2	1:E:101:ASP:H	1.81	0.45
1:G:3:GLN:HB2	1:G:25:THR:CG2	2.46	0.45
1:C:70:PHE:CD1	1:C:81:MET:HG3	2.51	0.45
1:C:60:TYR:CE2	1:C:70:PHE:CD2	3.04	0.45
1:E:260:PHE:HB3	1:E:263:VAL:CG2	2.47	0.45
1:G:77:ASN:ND2	2:G:348:HOH:O	2.48	0.45
1:E:231:HIS:ND1	1:E:232:SER:N	2.64	0.45
1:A:10:GLU:HG3	1:A:18:LEU:HD12	1.99	0.45
1:A:6:GLN:H	1:A:114:GLN:NE2	2.12	0.45
1:G:237:SER:HB3	1:G:296:SER:HB2	1.97	0.45
1:G:267:PHE:CE1	1:G:280:ILE:HG12	2.51	0.45
1:E:12:MET:CG	1:E:18:LEU:HD13	2.47	0.45
1:C:32:TYR:CD2	1:C:98:ARG:HD3	2.51	0.45
1:G:252:LEU:HD11	1:G:291:TYR:HE2	1.81	0.45
1:E:35:GLU:O	1:E:96:CYS:HA	2.16	0.45
1:A:259:ARG:HD2	1:A:263:VAL:HG22	1.99	0.45
1:G:76:SER:O	1:G:77:ASN:HB2	2.17	0.45
1:C:24:THR:OG1	1:C:29:PHE:CD1	2.69	0.45
1:C:266:ARG:O	1:C:280:ILE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:GLN:O	1:G:274:THR:HG22	2.17	0.45
1:A:20:ILE:HD11	1:A:81:MET:HE3	1.98	0.45
1:E:233:ASN:HD21	1:E:235:ASN:HB2	1.81	0.45
1:E:20:ILE:HD11	1:E:81:MET:CE	2.45	0.45
1:C:89:GLU:CG	2:C:345:HOH:O	2.64	0.45
1:A:13:LYS:HD3	1:A:121:SER:OG	2.17	0.44
1:A:241:TYR:HE1	1:A:294:SER:HG	1.64	0.44
1:G:100:GLU:HA	1:G:107:TYR:HA	1.99	0.44
1:E:2:VAL:HA	1:E:26:GLY:HA3	1.98	0.44
1:G:21:SER:HB3	1:G:80:TYR:CE1	2.52	0.44
1:C:100:GLU:HA	1:C:107:TYR:HA	2.00	0.44
1:C:60:TYR:CE2	1:C:70:PHE:CE2	3.06	0.44
1:C:233:ASN:HD21	1:C:235:ASN:H	1.65	0.44
1:A:18:LEU:HD23	1:A:83:LEU:HD12	1.97	0.44
1:E:236:THR:O	1:E:255:LYS:HA	2.18	0.44
1:C:206:GLN:HA	1:C:222:SER:O	2.17	0.44
1:A:19:LYS:HA	1:A:81:MET:O	2.18	0.44
1:A:300:PRO:O	1:A:302:THR:HG23	2.17	0.44
1:A:33:TRP:CE3	1:A:50:LYS:HE2	2.53	0.44
1:E:33:TRP:CE3	1:E:50:LYS:CE	3.01	0.43
1:C:24:THR:OG1	1:C:29:PHE:HD1	2.01	0.43
1:A:301:PHE:C	1:A:301:PHE:CD1	2.92	0.43
1:G:285:ALA:O	1:G:288:LEU:HG	2.18	0.43
1:A:242:LEU:HD13	1:A:291:TYR:CE1	2.53	0.43
1:G:29:PHE:CE1	1:G:77:ASN:O	2.71	0.43
1:A:242:LEU:HD13	1:A:291:TYR:CZ	2.53	0.43
1:G:35:GLU:O	1:G:96:CYS:HA	2.19	0.43
1:E:292:PHE:HD1	1:E:304:GLY:O	2.02	0.43
1:A:105:TYR:HE1	2:A:356:HOH:O	2.01	0.43
1:A:114:GLN:N	1:A:114:GLN:NE2	2.57	0.43
1:A:244:LYS:H	1:A:250:LYS:HZ1	1.65	0.43
1:E:94:TYR:O	1:E:115:GLY:HA2	2.19	0.43
1:G:12:MET:CG	1:G:18:LEU:HD13	2.49	0.43
1:G:225:SER:OG	1:G:274:THR:HA	2.19	0.43
1:C:33:TRP:CE3	1:C:50:LYS:HG3	2.54	0.43
1:G:107:TYR:CD1	1:G:107:TYR:C	2.90	0.43
1:C:220:SER:HA	1:C:278:LEU:O	2.19	0.43
1:A:224:ARG:NH2	1:E:212:PRO:HG2	2.33	0.43
1:C:48:ILE:HG23	1:C:64:PHE:CG	2.53	0.43
1:E:233:ASN:ND2	1:E:233:ASN:C	2.72	0.43
1:A:47:TRP:HH2	1:A:59:THR:HG22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LEU:HA	1:C:294:SER:O	2.19	0.43
1:A:103:TYR:O	1:A:104:ALA:HB3	2.19	0.42
1:C:48:ILE:HG23	1:C:64:PHE:CB	2.49	0.42
1:G:12:MET:HG3	1:G:18:LEU:HD13	2.02	0.42
1:C:51:ILE:HG13	1:C:58:ASN:OD1	2.19	0.42
1:C:53:PRO:HB3	1:C:74:THR:HG22	2.00	0.42
1:C:89:GLU:HG3	2:C:345:HOH:O	2.19	0.42
1:E:39:GLN:HG2	1:E:45:LEU:CD2	2.39	0.42
1:A:18:LEU:O	1:A:82:GLN:HA	2.19	0.42
1:E:81:MET:HB3	1:E:81:MET:HE3	1.83	0.42
1:E:40:ARG:HA	1:E:41:PRO:HD3	1.79	0.42
1:G:61:ASN:O	1:G:62:ASP:C	2.57	0.42
1:A:239:HIS:CD2	1:C:108:VAL:HG22	2.55	0.42
1:E:242:LEU:HD12	1:E:243:LYS:N	2.35	0.42
1:C:237:SER:HB3	1:C:296:SER:HB2	2.00	0.42
1:E:202:ILE:CD1	1:E:227:GLN:OE1	2.67	0.42
1:E:3:GLN:O	1:E:24:THR:HA	2.20	0.42
1:E:48:ILE:HG22	1:E:70:PHE:HZ	1.85	0.42
1:C:284:GLU:OE1	1:C:284:GLU:HA	2.19	0.42
1:E:47:TRP:CE3	1:E:61:ASN:HB2	2.55	0.42
1:E:18:LEU:HD21	1:E:83:LEU:HD12	2.00	0.42
1:C:2:VAL:HB	1:C:27:TYR:HD1	1.85	0.42
1:C:110:ASP:OD1	1:C:111:TYR:N	2.50	0.42
1:G:86:LEU:HA	1:G:90:ASP:OD2	2.19	0.42
1:C:33:TRP:CD2	1:C:50:LYS:HE2	2.55	0.42
1:G:40:ARG:HG2	1:G:41:PRO:HD2	2.02	0.42
1:A:4:LEU:O	1:A:113:GLY:HA2	2.20	0.42
1:E:74:THR:O	1:E:76:SER:N	2.53	0.42
1:A:33:TRP:CE3	1:A:50:LYS:HG3	2.55	0.42
1:E:231:HIS:CE1	1:E:232:SER:OG	2.73	0.42
1:A:29:PHE:CE2	1:A:53:PRO:HB3	2.54	0.42
1:G:244:LYS:H	1:G:250:LYS:NZ	2.16	0.42
1:E:14:PRO:HG3	1:E:120:VAL:HG12	2.02	0.42
1:E:93:VAL:HG11	1:E:95:TYR:CZ	2.54	0.42
2:A:364:HOH:O	1:C:301:PHE:HB2	2.20	0.42
1:E:23:LYS:HG3	1:E:78:ILE:CG1	2.39	0.41
1:G:73:ASP:OD1	1:G:75:SER:HB3	2.20	0.41
1:G:33:TRP:NE1	1:G:52:LEU:HD22	2.35	0.41
1:G:18:LEU:HD23	1:G:83:LEU:HD12	2.02	0.41
1:E:4:LEU:HG	1:E:24:THR:HG22	2.03	0.41
1:E:18:LEU:HD23	1:E:83:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:LEU:HD23	1:G:225:SER:HA	2.02	0.41
1:E:97:ALA:HA	1:E:111:TYR:O	2.20	0.41
1:G:294:SER:HA	1:G:302:THR:O	2.20	0.41
1:G:4:LEU:HD23	1:G:4:LEU:N	2.34	0.41
1:A:239:HIS:HA	1:A:253:ILE:O	2.20	0.41
1:A:220:SER:HA	1:A:278:LEU:O	2.20	0.41
1:E:2:VAL:HG22	1:E:111:TYR:CG	2.55	0.41
1:A:32:TYR:CD1	1:A:98:ARG:HD3	2.56	0.41
1:E:98:ARG:HD2	2:E:319:HOH:O	2.21	0.41
1:C:19:LYS:HG3	1:C:80:TYR:HB3	2.03	0.41
1:G:114:GLN:HG2	1:G:114:GLN:O	2.20	0.41
1:E:242:LEU:HD21	1:E:244:LYS:HD2	2.02	0.41
1:C:97:ALA:HA	1:C:111:TYR:O	2.20	0.41
1:G:3:GLN:H	1:G:25:THR:HG22	1.86	0.41
1:C:6:GLN:N	1:C:114:GLN:HE22	2.18	0.40
1:C:10:GLU:HB3	1:C:12:MET:CE	2.51	0.40
1:E:14:PRO:HD3	1:E:121:SER:O	2.21	0.40
1:E:6:GLN:HA	1:E:21:SER:O	2.21	0.40
1:G:70:PHE:CD1	1:G:81:MET:HG3	2.54	0.40
1:A:239:HIS:CD2	1:A:255:LYS:H	2.39	0.40
1:C:112:TRP:CD1	1:C:112:TRP:N	2.88	0.40
1:C:9:THR:HB	1:C:117:THR:O	2.21	0.40
1:C:2:VAL:HG22	1:C:111:TYR:CD1	2.56	0.40
1:G:50:LYS:HG2	1:G:59:THR:HB	2.04	0.40
1:E:28:ILE:O	1:E:31:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236/238 (99%)	216 (92%)	18 (8%)	2 (1%)	24	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	236/238 (99%)	215 (91%)	16 (7%)	5 (2%)	9	16
1	E	236/238 (99%)	215 (91%)	16 (7%)	5 (2%)	9	16
1	G	236/238 (99%)	209 (89%)	20 (8%)	7 (3%)	5	8
All	All	944/952 (99%)	855 (91%)	70 (7%)	19 (2%)	9	18

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	124	GLY
1	E	85	SER
1	E	256	VAL
1	A	85	SER
1	C	55	GLY
1	C	74	THR
1	E	100	GLU
1	G	85	SER
1	G	121	SER
1	G	255	LYS
1	C	56	GLY
1	C	102	TYR
1	E	29	PHE
1	E	75	SER
1	G	62	ASP
1	G	124	GLY
1	G	29	PHE
1	G	273	GLY
1	A	256	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/203 (100%)	182 (90%)	21 (10%)	9	16
1	C	203/203 (100%)	182 (90%)	21 (10%)	9	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	203/203 (100%)	179 (88%)	24 (12%)	6	12
1	G	203/203 (100%)	176 (87%)	27 (13%)	5	8
All	All	812/812 (100%)	719 (88%)	93 (12%)	7	12

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	18	LEU
1	A	20	ILE
1	A	30	SER
1	A	81	MET
1	A	101	ASP
1	A	107	TYR
1	A	114	GLN
1	A	226	SER
1	A	239	HIS
1	A	248	SER
1	A	250	LYS
1	A	253	ILE
1	A	261	SER
1	A	263	VAL
1	A	278	LEU
1	A	286	GLU
1	A	296	SER
1	A	301	PHE
1	A	310	GLU
1	A	311	LEU
1	C	2	VAL
1	C	7	SER
1	C	9	THR
1	C	16	ARG
1	C	17	SER
1	C	20	ILE
1	C	39	GLN
1	C	53	PRO
1	C	81	MET
1	C	107	TYR
1	C	114	GLN
1	C	214	SER
1	C	226	SER

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Mol	Chain	Res	Type
1	C	233	ASN
1	C	238	LEU
1	C	257	SER
1	C	261	SER
1	C	265	ASP
1	C	268	SER
1	C	278	LEU
1	C	286	GLU
1	E	2	VAL
1	E	7	SER
1	E	9	THR
1	E	16	ARG
1	E	18	LEU
1	E	39	GLN
1	E	53	PRO
1	E	57	SER
1	E	58	ASN
1	E	81	MET
1	E	85	SER
1	E	107	TYR
1	E	114	GLN
1	E	208	PRO
1	E	232	SER
1	E	233	ASN
1	E	239	HIS
1	E	250	LYS
1	E	257	SER
1	E	264	PRO
1	E	268	SER
1	E	270	SER
1	E	278	LEU
1	E	286	GLU
1	G	2	VAL
1	G	5	GLN
1	G	7	SER
1	G	18	LEU
1	G	23	LYS
1	G	25	THR
1	G	31	ASN
1	G	35	GLU
1	G	52	LEU
1	G	71	THR

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Mol	Chain	Res	Type
1	G	75	SER
1	G	81	MET
1	G	101	ASP
1	G	107	TYR
1	G	114	GLN
1	G	127	SER
1	G	226	SER
1	G	235	ASN
1	G	236	THR
1	G	238	LEU
1	G	239	HIS
1	G	245	PRO
1	G	248	SER
1	G	250	LYS
1	G	268	SER
1	G	278	LEU
1	G	286	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	239	HIS
1	C	114	GLN
1	C	218	GLN
1	C	233	ASN
1	C	239	HIS
1	E	218	GLN
1	E	233	ASN
1	E	235	ASN
1	E	239	HIS
1	G	114	GLN
1	G	218	GLN
1	G	239	HIS

### 5.3.3 RNA ⓘ

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.