



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2021 – 02:09 PM JST

PDB ID : 6LYS  
Title : Structure of the BAM complex  
Authors : Xiao, L.; Huang, Y.  
Deposited on : 2020-02-15  
Resolution : 3.05 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
Xtriage (Phenix)	:	1.13
EDS	:	2.16
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)	:	2.16

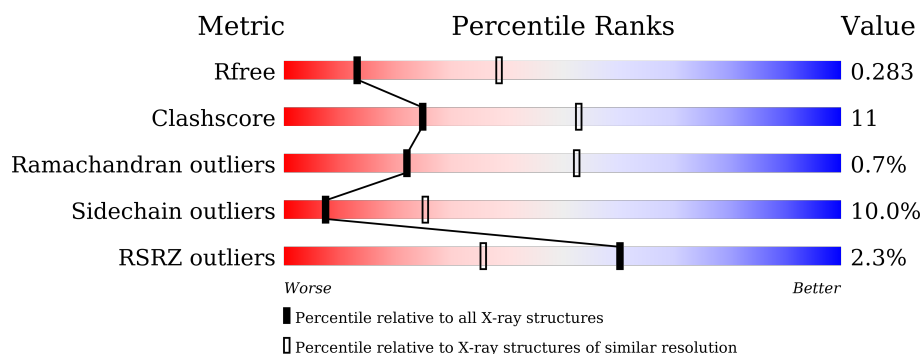
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 of 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	810	<div> <div>0%</div> <div> <div>72%</div> <div>23%</div> <div>5%</div> </div> <div>• •</div> </div>
2	B	400	<div> <div>0%</div> <div> <div>57%</div> <div>26%</div> <div>5%</div> <div>12%</div> </div> </div>
3	D	245	<div> <div>2%</div> <div> <div>60%</div> <div>22%</div> <div>15%</div> </div> <div>•</div> </div>
4	E	119	<div> <div>3%</div> <div> <div>54%</div> <div>12%</div> <div>30%</div> </div> <div>•</div> </div>
5	C	344	<div> <div>5%</div> <div> <div>35%</div> <div>8%</div> <div>55%</div> </div> <div>•</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12196 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	786	Total	C	N	O	S	0	0	0
			6152	3882	1033	1221	16			

- Molecule 2 is a protein called Outer membrane protein assembly factor BamB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	351	Total	C	N	O	S	0	0	0
			2607	1637	448	516	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	393	TRP	-	expression tag	UNP P77774
B	394	SER	-	expression tag	UNP P77774
B	395	HIS	-	expression tag	UNP P77774
B	396	PRO	-	expression tag	UNP P77774
B	397	GLN	-	expression tag	UNP P77774
B	398	PHE	-	expression tag	UNP P77774
B	399	GLU	-	expression tag	UNP P77774
B	400	LYS	-	expression tag	UNP P77774

- Molecule 3 is a protein called Outer membrane protein assembly factor BamD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	208	Total	C	N	O	S	0	0	0
			1682	1057	296	322	7			

- Molecule 4 is a protein called Outer membrane protein assembly factor BamE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	83	Total	C	N	O	S	0	0	0
			645	405	112	126	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	HIS	-	expression tag	UNP P0A937
E	115	HIS	-	expression tag	UNP P0A937
E	116	HIS	-	expression tag	UNP P0A937
E	117	HIS	-	expression tag	UNP P0A937
E	118	HIS	-	expression tag	UNP P0A937
E	119	HIS	-	expression tag	UNP P0A937

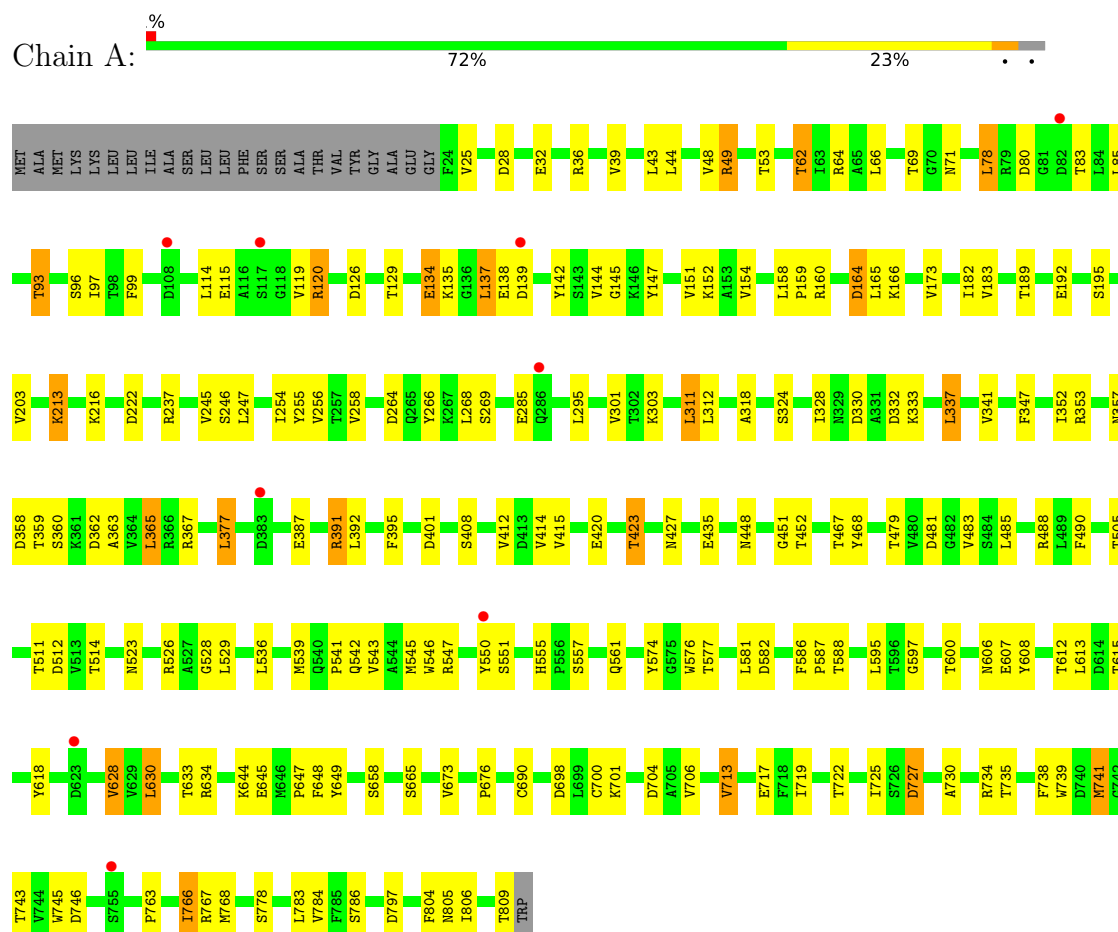
- Molecule 5 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	154	Total	C	N	O	S	1	0	0
			1110	694	194	219	3			

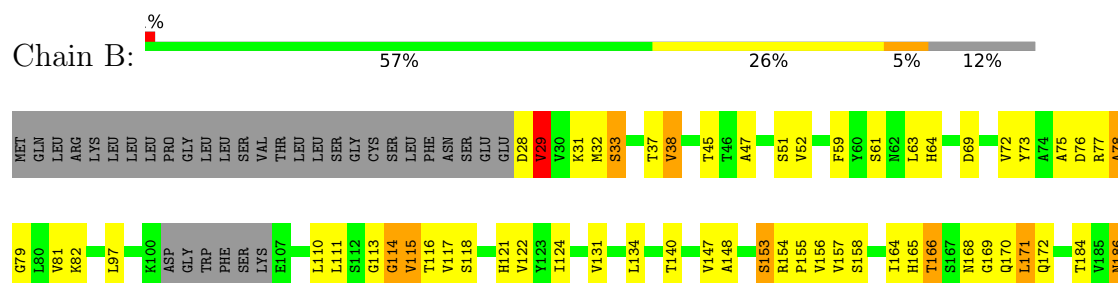
### 3 Residue-property plots

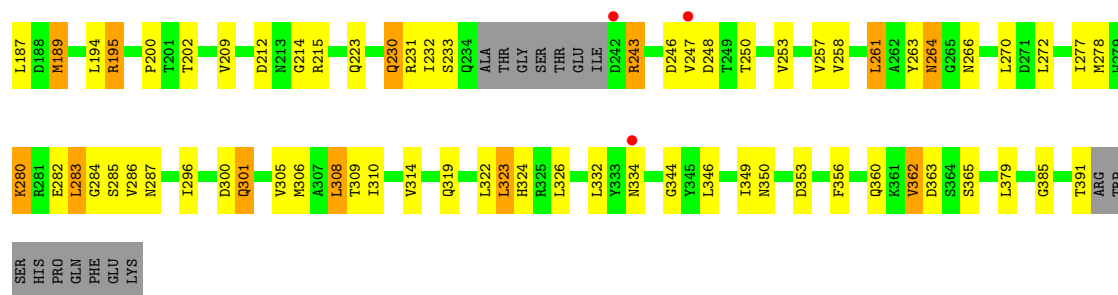
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Outer membrane protein assembly factor BamA



- Molecule 2: Outer membrane protein assembly factor BamB





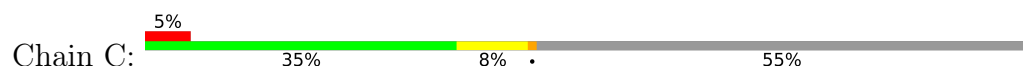
• Molecule 3: Outer membrane protein assembly factor BamD



• Molecule 4: Outer membrane protein assembly factor BamE



• Molecule 5: Outer membrane protein assembly factor BamC



ARG  
SER  
SER  
LEU  
GLN  
PHE  
ILE  
ASP  
PRO  
LYS  
GLY  
HIS  
THR  
LEU  
THR  
GLN  
SER  
GLN  
ASN  
ASP  
ALA  
LEU  
VAL  
ALA  
VAL  
PHE  
GLN  
ALA  
ALA  
PHE  
SER  
LYS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.07Å 117.07Å 429.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.05 10.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	96.4 (10.00-3.05) 99.7 (10.00-3.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.243 , 0.284 0.247 , 0.283	Depositor DCC
$R_{free}$ test set	2790 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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

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	0.63	0/6295	0.77	0/8554
2	B	0.66	0/2652	0.88	4/3622 (0.1%)
3	D	0.63	0/1719	0.73	0/2336
4	E	0.64	0/659	0.76	0/899
5	C	0.69	0/1127	0.83	0/1541
All	All	0.64	0/12452	0.80	4/16952 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	78	ALA	N-CA-C	-13.68	74.08	111.00
2	B	79	GLY	N-CA-C	8.30	133.85	113.10
2	B	264	ASN	CB-CA-C	-7.73	94.94	110.40
2	B	29	VAL	CB-CA-C	-5.19	101.54	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	248	ASP	Peptide

## 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	6152	0	5804	114	0
2	B	2607	0	2541	83	0
3	D	1682	0	1624	41	0
4	E	645	0	625	12	0
5	C	1110	0	1031	22	0
All	All	12196	0	11625	256	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 (256) 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:B:64:HIS:O	2:B:115:VAL:HG22	1.72	0.89
2:B:76:ASP:O	2:B:78:ALA:O	1.94	0.85
2:B:243:ARG:NE	2:B:243:ARG:O	2.08	0.85
2:B:77:ARG:C	2:B:78:ALA:O	2.01	0.84
1:A:547:ARG:NH2	1:A:746:ASP:OD1	2.12	0.81
3:D:92:ILE:HG21	3:D:112:ARG:HB3	1.64	0.80
1:A:743:THR:HG22	1:A:766:ILE:HA	1.62	0.79
2:B:284:GLY:O	2:B:301:GLN:HG3	1.84	0.78
1:A:318:ALA:HB2	1:A:377:LEU:HD21	1.66	0.77
1:A:43:LEU:O	1:A:49:ARG:NH2	2.21	0.74
2:B:33:SER:HB2	2:B:323:LEU:O	1.88	0.74
1:A:542:GLN:HE22	1:A:706:VAL:HG21	1.53	0.72
2:B:38:VAL:HG21	2:B:356:PHE:HB2	1.73	0.71
2:B:296:ILE:HG13	2:B:310:ILE:HG22	1.72	0.70
2:B:29:VAL:HG12	2:B:29:VAL:O	1.91	0.69
2:B:200:PRO:HB3	2:B:209:VAL:HG12	1.76	0.68
1:A:745:TRP:CD2	1:A:763:PRO:HB3	2.30	0.66
1:A:347:PHE:HB2	1:A:377:LEU:HD22	1.76	0.66
2:B:115:VAL:HG12	2:B:124:ILE:HD11	1.76	0.66
4:E:55:VAL:HG21	4:E:95:PHE:HZ	1.61	0.66
1:A:805:ASN:OD1	1:A:809:THR:OG1	2.12	0.66
2:B:284:GLY:O	2:B:301:GLN:CD	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:LEU:HG	1:A:806:ILE:HD13	1.78	0.65
3:D:165:LYS:O	3:D:168:VAL:HG12	1.97	0.65
1:A:363:ALA:O	1:A:367:ARG:HG2	1.97	0.64
2:B:284:GLY:O	2:B:301:GLN:CG	2.44	0.64
5:C:166:GLN:C	5:C:168:ARG:N	2.51	0.64
1:A:160:ARG:NH1	3:D:61:ARG:O	2.31	0.64
2:B:283:LEU:HD13	2:B:306:MET:HE1	1.78	0.63
5:C:188:LEU:HD11	5:C:191:LEU:HB2	1.80	0.63
2:B:344:GLY:HA3	2:B:363:ASP:O	1.99	0.63
1:A:266:TYR:CZ	1:A:328:ILE:HD11	2.33	0.63
1:A:360:SER:HA	1:A:451:GLY:HA3	1.80	0.62
1:A:311:LEU:HD12	1:A:311:LEU:C	2.19	0.62
1:A:541:PRO:HA	1:A:546:TRP:CZ3	2.35	0.61
2:B:171:LEU:HD22	2:B:209:VAL:HG11	1.83	0.61
1:A:324:SER:HB2	1:A:337:LEU:HD21	1.83	0.61
2:B:52:VAL:HG22	2:B:385:GLY:O	2.01	0.61
1:A:717:GLU:HG2	1:A:738:PHE:HB3	1.84	0.60
4:E:67:PRO:HB2	5:C:59:PRO:HG3	1.83	0.60
2:B:75:ALA:HB2	2:B:81:VAL:HG12	1.84	0.60
2:B:131:VAL:HG21	2:B:164:ILE:HG13	1.83	0.60
5:C:130:VAL:HG22	5:C:215:ILE:HD11	1.83	0.60
3:D:186:THR:HG21	3:D:217:LEU:HD23	1.85	0.59
3:D:206:PRO:O	5:C:50:LEU:HD11	2.03	0.59
3:D:167:LEU:HD13	5:C:67:ILE:HG22	1.82	0.59
2:B:277:ILE:HG21	2:B:280:LYS:HE3	1.84	0.58
1:A:182:ILE:HG12	1:A:258:VAL:HG22	1.86	0.58
2:B:64:HIS:O	2:B:115:VAL:CG2	2.48	0.58
2:B:261:LEU:HD22	2:B:285:SER:HB3	1.86	0.58
3:D:198:VAL:HG11	3:D:218:MET:HB2	1.84	0.57
5:C:171:TYR:CE1	5:C:188:LEU:HD23	2.39	0.57
1:A:318:ALA:CB	1:A:377:LEU:HD21	2.32	0.57
1:A:139:ASP:HA	1:A:142:TYR:HD2	1.68	0.57
2:B:117:VAL:HG22	2:B:122:VAL:HG12	1.86	0.57
1:A:324:SER:HB2	1:A:337:LEU:CD2	2.35	0.57
1:A:628:VAL:HG22	1:A:719:ILE:HD12	1.87	0.56
1:A:347:PHE:HB2	1:A:377:LEU:CD2	2.36	0.56
2:B:158:SER:OG	2:B:202:THR:HG21	2.06	0.56
2:B:214:GLY:HA3	2:B:233:SER:HB3	1.88	0.56
1:A:66:LEU:O	1:A:69:THR:HB	2.06	0.55
2:B:284:GLY:O	2:B:301:GLN:OE1	2.24	0.55
2:B:113:GLY:O	2:B:114:GLY:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:HG12	1:A:53:THR:HG22	1.89	0.54
2:B:169:GLY:O	2:B:187:LEU:HB2	2.07	0.54
1:A:192:GLU:O	1:A:195:SER:HB3	2.08	0.54
2:B:350:ASN:ND2	2:B:353:ASP:OD1	2.34	0.54
2:B:47:ALA:HB2	2:B:391:THR:HG23	1.90	0.54
1:A:634:ARG:HB3	1:A:713:VAL:HG13	1.90	0.54
2:B:258:VAL:HG22	2:B:270:LEU:HB2	1.89	0.54
3:D:225:MET:O	4:E:88:GLN:NE2	2.39	0.54
1:A:114:LEU:HB3	1:A:119:VAL:HG23	1.88	0.54
1:A:266:TYR:CE2	1:A:328:ILE:HD11	2.42	0.54
2:B:153:SER:OG	2:B:165:HIS:O	2.26	0.54
5:C:130:VAL:HG21	5:C:175:VAL:HG21	1.89	0.54
1:A:551:SER:OG	1:A:645:GLU:HG3	2.07	0.54
2:B:52:VAL:HG12	2:B:82:LYS:HD2	1.89	0.54
1:A:618:TYR:CZ	1:A:630:LEU:HD12	2.43	0.53
2:B:147:VAL:HG13	2:B:172:GLN:OE1	2.08	0.53
2:B:305:VAL:HG11	2:B:349:ILE:CD1	2.38	0.53
3:D:164:THR:HA	3:D:167:LEU:HD11	1.90	0.53
2:B:230:GLN:NE2	2:B:231:ARG:O	2.42	0.53
3:D:191:TRP:O	3:D:195:VAL:HG12	2.09	0.52
2:B:305:VAL:HG11	2:B:349:ILE:HD12	1.91	0.52
3:D:209:GLN:NE2	3:D:213:ASP:OD1	2.43	0.52
1:A:353:ARG:HB2	1:A:415:VAL:HG12	1.92	0.52
4:E:104:ILE:HG13	4:E:104:ILE:O	2.08	0.52
4:E:46:ILE:HG22	4:E:55:VAL:HG12	1.92	0.52
2:B:194:LEU:O	2:B:247:VAL:HG21	2.10	0.52
1:A:360:SER:HB3	1:A:448:ASN:HD21	1.75	0.51
1:A:96:SER:OG	1:A:164:ASP:OD1	2.25	0.51
1:A:595:LEU:HB2	1:A:613:LEU:HD12	1.91	0.51
3:D:169:PHE:CG	5:C:42:LEU:HD12	2.45	0.51
3:D:27:VAL:HG22	3:D:28:PRO:HD2	1.92	0.51
1:A:542:GLN:HE21	1:A:545:MET:H	1.58	0.51
2:B:77:ARG:HE	2:B:110:LEU:HD12	1.75	0.51
1:A:551:SER:HB3	1:A:644:LYS:HA	1.93	0.51
2:B:76:ASP:C	2:B:78:ALA:O	2.48	0.51
2:B:309:THR:HG22	2:B:314:VAL:HG22	1.92	0.51
3:D:192:VAL:HA	4:E:64:MET:HE1	1.91	0.51
2:B:246:ASP:HB3	2:B:263:TYR:O	2.11	0.51
1:A:423:THR:HG21	1:A:448:ASN:HB3	1.93	0.51
1:A:468:TYR:HE1	1:A:490:PHE:HB2	1.75	0.51
2:B:323:LEU:CD2	2:B:324:HIS:CE1	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:167:LEU:HD13	5:C:67:ILE:CG2	2.41	0.51
1:A:582:ASP:OD2	1:A:588:THR:HG22	2.11	0.51
1:A:145:GLY:HA3	1:A:213:LYS:CE	2.41	0.50
1:A:138:GLU:HB2	1:A:151:VAL:HG22	1.94	0.50
1:A:523:ASN:HD22	1:A:576:TRP:HE1	1.58	0.50
1:A:134:GLU:HB3	1:A:151:VAL:HG23	1.94	0.50
2:B:253:VAL:HB	2:B:258:VAL:HG12	1.94	0.49
5:C:43:GLU:O	5:C:43:GLU:HG2	2.12	0.49
1:A:48:VAL:HG23	1:A:62:THR:HG21	1.93	0.49
1:A:154:VAL:HG22	1:A:166:LYS:HG2	1.95	0.49
1:A:550:TYR:HE1	1:A:555:HIS:HA	1.76	0.49
1:A:543:VAL:HG13	1:A:673:VAL:HG23	1.95	0.49
1:A:745:TRP:CE3	1:A:763:PRO:HB3	2.46	0.49
1:A:32:GLU:HB3	5:C:160:ARG:HD2	1.95	0.49
2:B:115:VAL:HG12	2:B:124:ILE:CD1	2.42	0.49
1:A:359:THR:O	3:D:135:ARG:NH1	2.46	0.48
1:A:526:ARG:NH2	1:A:577:THR:OG1	2.44	0.48
1:A:727:ASP:OD1	1:A:727:ASP:N	2.46	0.48
1:A:255:TYR:CD1	2:B:195:ARG:HD2	2.48	0.48
2:B:212:ASP:HA	2:B:247:VAL:HA	1.96	0.48
1:A:767:ARG:HD2	1:A:797:ASP:OD2	2.13	0.48
2:B:118:SER:HB3	2:B:157:VAL:HG11	1.94	0.48
1:A:78:LEU:HD22	1:A:78:LEU:H	1.78	0.48
1:A:237:ARG:HD2	1:A:328:ILE:HD13	1.95	0.48
3:D:172:ASP:HA	3:D:175:ALA:HB3	1.95	0.47
3:D:30:ASN:HB3	3:D:31:PRO:HD2	1.94	0.47
1:A:36:ARG:HD3	1:A:93:THR:HG21	1.94	0.47
2:B:75:ALA:CB	2:B:81:VAL:HG12	2.44	0.47
1:A:725:ILE:HD13	1:A:730:ALA:HA	1.96	0.47
2:B:111:LEU:HD13	2:B:124:ILE:HG21	1.97	0.47
3:D:194:VAL:HG22	3:D:221:ALA:HB2	1.96	0.47
1:A:318:ALA:HB2	1:A:377:LEU:CD2	2.39	0.47
1:A:514:THR:HG22	1:A:528:GLY:HA3	1.96	0.47
1:A:387:GLU:OE2	1:A:391:ARG:NH2	2.43	0.47
1:A:479:THR:OG1	1:A:483:VAL:HG22	2.14	0.47
1:A:600:THR:HG21	1:A:607:GLU:HA	1.97	0.47
5:C:209:THR:HG22	5:C:213:ASN:ND2	2.29	0.47
1:A:647:PRO:HB3	1:A:649:TYR:CE2	2.50	0.47
1:A:615:THR:HB	1:A:633:THR:OG1	2.15	0.47
2:B:29:VAL:O	2:B:29:VAL:CG1	2.61	0.46
1:A:137:LEU:HD12	1:A:151:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:SER:OG	2:B:286:VAL:N	2.48	0.46
2:B:72:VAL:HG22	2:B:379:LEU:HD11	1.98	0.46
1:A:134:GLU:O	1:A:138:GLU:HB3	2.16	0.46
1:A:48:VAL:HG23	1:A:62:THR:CG2	2.44	0.46
2:B:59:PHE:HB3	2:B:77:ARG:NH1	2.30	0.46
5:C:127:TRP:HB3	5:C:128:PRO:HD3	1.98	0.46
1:A:481:ASP:OD1	3:D:188:ARG:NH2	2.47	0.46
1:A:311:LEU:HD12	1:A:312:LEU:N	2.30	0.46
1:A:743:THR:CG2	1:A:766:ILE:HG22	2.45	0.46
1:A:743:THR:CG2	1:A:766:ILE:HA	2.41	0.46
4:E:80:GLN:HB2	4:E:86:VAL:HG12	1.99	0.45
3:D:174:LEU:HD12	3:D:205:TYR:CE1	2.50	0.45
1:A:158:LEU:HB3	1:A:159:PRO:HD2	1.99	0.45
2:B:116:THR:HG21	2:B:155:PRO:O	2.17	0.45
1:A:44:LEU:O	1:A:44:LEU:HD22	2.16	0.45
2:B:115:VAL:CG1	2:B:124:ILE:HD11	2.46	0.45
2:B:223:GLN:N	2:B:223:GLN:OE1	2.50	0.45
3:D:117:MET:HG3	3:D:170:LEU:HD21	1.99	0.45
2:B:306:MET:HE3	2:B:308:LEU:HD11	1.98	0.45
2:B:64:HIS:NE2	2:B:154:ARG:HD3	2.32	0.45
3:D:115:THR:O	3:D:119:LEU:HD13	2.16	0.45
1:A:142:TYR:HD1	1:A:147:TYR:HD1	1.64	0.45
1:A:488:ARG:O	1:A:511:THR:HA	2.16	0.45
5:C:134:LEU:HD22	5:C:211:MET:HE3	1.98	0.45
5:C:211:MET:O	5:C:215:ILE:HG22	2.17	0.45
2:B:189:MET:HE3	2:B:212:ASP:HB2	1.99	0.45
3:D:194:VAL:CG2	3:D:221:ALA:HB2	2.47	0.45
2:B:186:ASN:HD22	2:B:186:ASN:C	2.20	0.45
2:B:319:GLN:NE2	2:B:356:PHE:CE2	2.85	0.45
1:A:784:VAL:O	1:A:804:PHE:HA	2.17	0.44
3:D:167:LEU:HA	3:D:170:LEU:HB2	1.99	0.44
2:B:266:ASN:OD1	2:B:282:GLU:HA	2.17	0.44
1:A:365:LEU:HD23	1:A:395:PHE:CZ	2.52	0.44
1:A:600:THR:HG22	1:A:608:TYR:O	2.17	0.44
2:B:246:ASP:CB	2:B:263:TYR:O	2.65	0.44
1:A:115:GLU:HG2	1:A:120:ARG:HB2	2.00	0.44
1:A:725:ILE:CD1	1:A:730:ALA:HA	2.48	0.44
1:A:766:ILE:O	1:A:766:ILE:HG13	2.17	0.44
1:A:357:ASN:HB3	1:A:365:LEU:HD21	1.99	0.44
1:A:536:LEU:HD22	1:A:648:PHE:CZ	2.53	0.44
5:C:207:TYR:HA	5:C:210:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:157:SER:O	3:D:160:THR:HG22	2.17	0.44
3:D:85:LEU:CD1	5:C:33:ARG:HG2	2.47	0.44
2:B:215:ARG:NH2	2:B:231:ARG:HD3	2.33	0.44
2:B:263:TYR:O	2:B:264:ASN:HB2	2.18	0.44
1:A:213:LYS:HA	1:A:213:LYS:HD2	1.60	0.43
1:A:739:TRP:HZ2	1:A:768:MET:HE2	1.84	0.43
1:A:741:MET:HA	1:A:767:ARG:O	2.19	0.43
3:D:194:VAL:O	3:D:198:VAL:HG12	2.18	0.43
3:D:99:ASN:HB3	3:D:102:HIS:HB2	2.00	0.43
1:A:586:PHE:CD2	1:A:734:ARG:HD3	2.54	0.43
2:B:258:VAL:CG2	2:B:270:LEU:HB2	2.49	0.43
3:D:84:ASP:HB3	3:D:87:LEU:HD12	2.01	0.43
3:D:147:PHE:CZ	3:D:166:ARG:HD3	2.54	0.43
4:E:91:LEU:HD12	4:E:106:ASN:HB3	2.00	0.43
1:A:126:ASP:OD1	1:A:129:THR:OG1	2.22	0.43
1:A:301:VAL:HG22	1:A:337:LEU:HD11	2.01	0.43
1:A:401:ASP:HB3	1:A:415:VAL:HG22	2.01	0.43
1:A:542:GLN:HE22	1:A:706:VAL:CG2	2.28	0.43
3:D:110:TYR:CD1	3:D:159:TYR:HB3	2.53	0.42
1:A:203:VAL:HG23	1:A:203:VAL:O	2.19	0.42
1:A:359:THR:HG22	1:A:420:GLU:OE1	2.19	0.42
1:A:255:TYR:CG	2:B:195:ARG:HD2	2.54	0.42
5:C:127:TRP:CH2	5:C:151:LEU:HD23	2.53	0.42
4:E:73:TRP:CD2	4:E:95:PHE:HE2	2.37	0.42
1:A:144:VAL:O	1:A:213:LYS:HE3	2.18	0.42
1:A:295:LEU:HA	1:A:295:LEU:HD23	1.83	0.42
2:B:148:ALA:HB1	2:B:170:GLN:HG3	2.01	0.42
2:B:156:VAL:HG21	2:B:200:PRO:O	2.19	0.42
2:B:97:LEU:HD11	2:B:134:LEU:HD11	2.01	0.42
2:B:97:LEU:HD21	2:B:134:LEU:HD21	2.01	0.42
3:D:232:GLU:HA	3:D:232:GLU:OE1	2.19	0.42
2:B:215:ARG:CZ	2:B:231:ARG:HD3	2.49	0.42
5:C:139:TYR:CE1	5:C:156:VAL:HG13	2.55	0.42
1:A:135:LYS:O	1:A:139:ASP:HB2	2.19	0.42
1:A:360:SER:HA	1:A:451:GLY:CA	2.49	0.42
1:A:574:TYR:CZ	1:A:597:GLY:HA3	2.55	0.42
4:E:101:LEU:HA	4:E:101:LEU:HD12	1.94	0.42
3:D:73:LEU:O	3:D:76:ILE:HG12	2.20	0.41
1:A:69:THR:CG2	1:A:71:ASN:ND2	2.83	0.41
2:B:117:VAL:HA	2:B:121:HIS:O	2.19	0.41
2:B:52:VAL:O	2:B:52:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:182:ALA:O	3:D:186:THR:HG22	2.21	0.41
1:A:435:GLU:OE1	1:A:665:SER:OG	2.39	0.41
2:B:257:VAL:HG12	2:B:278:MET:SD	2.60	0.41
3:D:214:ALA:O	3:D:217:LEU:HB2	2.20	0.41
3:D:195:VAL:HG13	4:E:64:MET:CE	2.50	0.41
1:A:97:ILE:HG22	1:A:99:PHE:CZ	2.55	0.41
2:B:73:TYR:CD2	2:B:122:VAL:HG11	2.55	0.41
2:B:148:ALA:HB3	2:B:166:THR:HG21	2.02	0.41
1:A:745:TRP:CE2	1:A:763:PRO:HB3	2.56	0.41
5:C:192:GLU:HA	5:C:197:PRO:HA	2.02	0.41
3:D:85:LEU:HB2	3:D:86:PRO:HD3	2.02	0.41
1:A:147:TYR:HE2	1:A:254:ILE:HD11	1.86	0.41
1:A:676:PRO:HG3	1:A:698:ASP:O	2.21	0.41
1:A:137:LEU:CD1	1:A:151:VAL:HG21	2.51	0.41
2:B:246:ASP:OD1	2:B:246:ASP:N	2.53	0.41
4:E:77:PHE:HB3	4:E:89:GLN:HG2	2.03	0.41
1:A:778:SER:OG	1:A:783:LEU:HD11	2.21	0.41
1:A:539:MET:HB3	1:A:545:MET:SD	2.61	0.40
3:D:178:GLU:O	3:D:181:VAL:HG22	2.21	0.40
1:A:362:ASP:O	1:A:365:LEU:HD12	2.21	0.40
1:A:722:THR:HG22	1:A:735:THR:OG1	2.21	0.40
2:B:232:ILE:HG22	2:B:277:ILE:HD11	2.03	0.40
2:B:283:LEU:CD1	2:B:306:MET:HE1	2.48	0.40
3:D:218:MET:HE3	3:D:234:VAL:HG21	2.02	0.40
2:B:350:ASN:HD22	2:B:353:ASP:CG	2.22	0.40
3:D:169:PHE:CD2	5:C:42:LEU:HD12	2.55	0.40
1:A:352:ILE:HA	1:A:414:VAL:O	2.22	0.40
1:A:581:LEU:HD22	1:A:587:PRO:HB3	2.03	0.40
2:B:172:GLN:HG2	2:B:184:THR:HG23	2.03	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	784/810 (97%)	735 (94%)	48 (6%)	1 (0%)	51	81
2	B	345/400 (86%)	311 (90%)	26 (8%)	8 (2%)	6	24
3	D	204/245 (83%)	197 (97%)	6 (3%)	1 (0%)	29	60
4	E	81/119 (68%)	75 (93%)	5 (6%)	1 (1%)	13	40
5	C	144/344 (42%)	126 (88%)	18 (12%)	0	100	100
All	All	1558/1918 (81%)	1444 (93%)	103 (7%)	11 (1%)	22	52

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	29	VAL
2	B	114	GLY
2	B	300	ASP
1	A	80	ASP
2	B	69	ASP
2	B	63	LEU
3	D	121	ASP
2	B	31	LYS
2	B	250	THR
2	B	362	VAL
4	E	70	THR

### 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	654/688 (95%)	587 (90%)	67 (10%)	7	24
2	B	278/329 (84%)	243 (87%)	35 (13%)	4	16
3	D	176/204 (86%)	165 (94%)	11 (6%)	18	45
4	E	72/101 (71%)	64 (89%)	8 (11%)	6	21
5	C	108/276 (39%)	100 (93%)	8 (7%)	13	39
All	All	1288/1598 (81%)	1159 (90%)	129 (10%)	7	25

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	39	VAL
1	A	49	ARG
1	A	62	THR
1	A	64	ARG
1	A	78	LEU
1	A	83	THR
1	A	85	LEU
1	A	93	THR
1	A	120	ARG
1	A	134	GLU
1	A	137	LEU
1	A	152	LYS
1	A	164	ASP
1	A	165	LEU
1	A	173	VAL
1	A	183	VAL
1	A	189	THR
1	A	213	LYS
1	A	216	LYS
1	A	222	ASP
1	A	245	VAL
1	A	246	SER
1	A	247	LEU
1	A	256	VAL
1	A	264	ASP
1	A	268	LEU
1	A	269	SER
1	A	285	GLU
1	A	303	LYS
1	A	311	LEU
1	A	330	ASP
1	A	332	ASP
1	A	333	LYS
1	A	337	LEU
1	A	341	VAL
1	A	358	ASP
1	A	365	LEU
1	A	377	LEU
1	A	391	ARG
1	A	392	LEU
1	A	408	SER

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Mol	Chain	Res	Type
1	A	412	VAL
1	A	423	THR
1	A	427	ASN
1	A	452	THR
1	A	467	THR
1	A	485	LEU
1	A	505	THR
1	A	512	ASP
1	A	529	LEU
1	A	557	SER
1	A	561	GLN
1	A	606	ASN
1	A	612	THR
1	A	628	VAL
1	A	630	LEU
1	A	658	SER
1	A	690	CYS
1	A	700	CYS
1	A	701	LYS
1	A	704	ASP
1	A	713	VAL
1	A	727	ASP
1	A	741	MET
1	A	766	ILE
1	A	786	SER
2	B	28	ASP
2	B	32	MET
2	B	33	SER
2	B	37	THR
2	B	38	VAL
2	B	45	THR
2	B	51	SER
2	B	61	SER
2	B	115	VAL
2	B	140	THR
2	B	153	SER
2	B	166	THR
2	B	168	ASN
2	B	171	LEU
2	B	186	ASN
2	B	189	MET
2	B	195	ARG

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Mol	Chain	Res	Type
2	B	230	GLN
2	B	243	ARG
2	B	261	LEU
2	B	272	LEU
2	B	280	LYS
2	B	283	LEU
2	B	287	ASN
2	B	301	GLN
2	B	308	LEU
2	B	322	LEU
2	B	323	LEU
2	B	326	LEU
2	B	332	LEU
2	B	334	ASN
2	B	346	LEU
2	B	360	GLN
2	B	362	VAL
2	B	365	SER
3	D	94	ARG
3	D	116	ASN
3	D	135	ARG
3	D	167	LEU
3	D	173	ARG
3	D	186	THR
3	D	194	VAL
3	D	195	VAL
3	D	205	TYR
3	D	212	ARG
3	D	228	ASN
4	E	63	LEU
4	E	70	THR
4	E	71	ASN
4	E	89	GLN
4	E	91	LEU
4	E	94	THR
4	E	104	ILE
4	E	106	ASN
5	C	33	ARG
5	C	43	GLU
5	C	62	SER
5	C	69	VAL
5	C	161	LEU

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Mol	Chain	Res	Type
5	C	162	ASP
5	C	210	GLU
5	C	215	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	A	259	ASN
1	A	542	GLN
2	B	186	ASN
2	B	225	GLN
2	B	229	GLN
3	D	47	ASN
3	D	89	GLN
3	D	116	ASN
5	C	124	ASN
5	C	182	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 monosaccharides 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 ⓘ

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	786/810 (97%)	-0.14	9 (1%) 80 60	69, 93, 122, 149	0
2	B	351/400 (87%)	-0.29	3 (0%) 84 66	72, 96, 117, 140	0
3	D	208/245 (84%)	-0.03	5 (2%) 59 34	73, 94, 139, 157	0
4	E	83/119 (69%)	-0.10	3 (3%) 42 21	74, 99, 131, 155	0
5	C	154/344 (44%)	0.59	16 (10%) 6 2	85, 140, 177, 199	1 (0%)
All	All	1582/1918 (82%)	-0.09	36 (2%) 60 36	69, 96, 144, 199	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	C	180	TYR	5.9
5	C	30	ARG	5.3
5	C	31	TYR	4.8
3	D	41	GLN	4.3
1	A	286	GLN	4.1
5	C	179	GLY	4.1
5	C	138	ASN	3.6
5	C	135	GLN	3.4
3	D	47	ASN	3.1
5	C	194	ALA	3.0
5	C	219	LEU	3.0
1	A	108	ASP	3.0
5	C	125	THR	2.9
1	A	383	ASP	2.9
3	D	34	GLU	2.9
3	D	44	GLN	2.8
5	C	115	SER	2.7
2	B	247	VAL	2.7
1	A	755	SER	2.6
5	C	124	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
4	E	83	HIS	2.5
1	A	82	ASP	2.5
2	B	334	ASN	2.5
1	A	139	ASP	2.5
3	D	138	GLN	2.5
5	C	113	THR	2.2
5	C	136	ALA	2.2
5	C	154	ASP	2.2
4	E	42	ASP	2.2
1	A	117	SER	2.2
4	E	40	ALA	2.1
1	A	550	TYR	2.1
5	C	128	PRO	2.1
1	A	623	ASP	2.1
5	C	203	SER	2.0
2	B	242	ASP	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 monosaccharides 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.