



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:23 PM GMT

PDB ID : 1IKN  
Title : IKAPPABALPHA/NF-KAPPABCOMPLEX  
Authors : Huxford, T.; Huang, D.-B.; Malek, S.; Ghosh, G.  
Deposited on : 1998-11-13  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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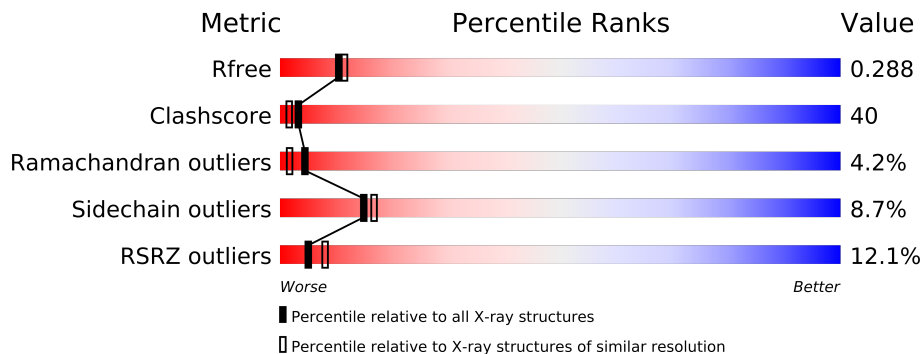
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	286	
2	C	119	
3	D	236	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4979 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (NF-KAPPA-B P65 SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	1
			2262	1405	422	424	11			

- Molecule 2 is a protein called PROTEIN (NF-KAPPA-B P50D SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	113	Total	C	N	O	S	0	0	1
			916	584	152	177	3			

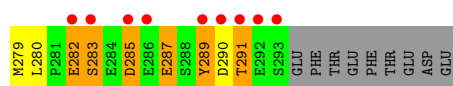
- Molecule 3 is a protein called PROTEIN (I-KAPPA-B-ALPHA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	216	Total	C	N	O	S	0	0	1
			1589	991	281	309	8			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total	O	0	0
			89	89		
4	C	53	Total	O	0	0
			53	53		
4	D	70	Total	O	0	0
			70	70		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.50Å 49.30Å 120.60Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30 24.88 – 2.25	Depositor EDS
% Data completeness (in resolution range)	74.2 (6.00-2.30) 77.2 (24.88-2.25)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.17 (at 2.26Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.223 , 0.277 0.238 , 0.288	Depositor DCC
$R_{free}$ test set	1300 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 74.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 25696 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.35	0/2313	0.63	1/3132 (0.0%)
2	C	0.44	0/936	0.67	0/1262
3	D	0.38	0/1616	0.66	0/2209
All	All	0.38	0/4865	0.65	1/6603 (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	19	PRO	N-CA-CB	5.28	109.63	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2262	0	2217	191	0
2	C	916	0	896	60	0
3	D	1589	0	1510	156	0
4	A	89	0	0	8	0
4	C	53	0	0	4	0
4	D	70	0	0	10	0
All	All	4979	0	4623	380	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 40.

All (380) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:122:LYS:HD2	1:A:122:LYS:H	1.16	1.05
3:D:105:ASN:HD22	3:D:114:PRO:HD2	1.23	1.01
1:A:87:PRO:HB2	1:A:121:VAL:HG11	1.47	0.97
1:A:79:LYS:HA	1:A:158:ARG:HD2	1.49	0.94
1:A:64:ASN:HB2	4:A:370:HOH:O	1.70	0.92
1:A:291:ASP:HB3	1:A:295:ARG:HB2	1.53	0.91
3:D:138:GLU:O	3:D:140:ARG:HG2	1.72	0.89
3:D:245:ARG:HA	3:D:245:ARG:NE	1.87	0.87
3:D:140:ARG:HD2	3:D:144:GLY:O	1.75	0.87
3:D:81:ALA:HB1	3:D:90:THR:HA	1.58	0.85
1:A:229:THR:HG22	4:A:373:HOH:O	1.77	0.84
3:D:143:ARG:HH22	3:D:150:LEU:HD21	1.42	0.83
2:C:352:LYS:HA	2:C:352:LYS:NZ	1.93	0.83
1:A:158:ARG:NH1	1:A:182:PRO:HD3	1.93	0.82
1:A:81:PRO:HB2	1:A:82:PRO:HD3	1.59	0.82
2:C:248:LEU:HD11	2:C:333:ARG:HG3	1.60	0.82
1:A:282:GLU:HG2	1:A:283:PRO:HD2	1.59	0.81
2:C:333:ARG:NH1	2:C:338:GLU:HB2	1.95	0.81
1:A:33:ARG:HB3	1:A:186:ASN:CG	2.01	0.81
2:C:324:PRO:HB2	2:C:346:LEU:HD11	1.61	0.81
3:D:172:LEU:HD13	3:D:173:HIS:N	1.94	0.81
1:A:131:SER:O	1:A:135:GLN:HG2	1.82	0.80
1:A:33:ARG:HG3	1:A:35:ARG:HH22	1.47	0.79
3:D:162:VAL:O	3:D:165:GLN:HG3	1.83	0.79
3:D:216:ASN:HD22	3:D:218:ARG:HE	1.30	0.79
3:D:210:ASN:HD21	3:D:242:ASP:H	1.31	0.79
3:D:169:THR:HA	3:D:174:SER:HB3	1.65	0.78
3:D:137:PRO:HG2	3:D:138:GLU:H	1.48	0.78
3:D:174:SER:HB2	4:D:348:HOH:O	1.83	0.78
3:D:138:GLU:C	3:D:139:LEU:HD23	2.04	0.78
1:A:290:PRO:HD3	4:A:381:HOH:O	1.82	0.78
2:C:343:LYS:HD3	4:D:304:HOH:O	1.83	0.78
2:C:274:GLN:HG3	4:C:115:HOH:O	1.82	0.77
2:C:261:THR:O	2:C:315:LYS:HG3	1.84	0.77
1:A:122:LYS:H	1:A:122:LYS:CD	1.94	0.77
1:A:32:MET:HA	1:A:33:ARG:NH2	2.01	0.76
1:A:33:ARG:HG2	1:A:35:ARG:HH12	1.51	0.76
1:A:122:LYS:HD2	1:A:122:LYS:N	2.00	0.75
3:D:114:PRO:HA	3:D:117:LEU:HD23	1.66	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:121:THR:HG22	3:D:123:GLN:HG3	1.69	0.75
1:A:187:ARG:HH12	1:A:220:GLN:NE2	1.84	0.74
2:C:249:LYS:HB3	2:C:271:ASP:OD1	1.87	0.74
1:A:194:LEU:HD22	1:A:279:GLU:HG3	1.69	0.74
3:D:185:THR:H	3:D:188:HIS:CD2	2.06	0.74
2:C:336:ASP:OD2	2:C:338:GLU:HG2	1.87	0.74
1:A:33:ARG:HB3	1:A:186:ASN:OD1	1.88	0.73
1:A:262:LEU:HD21	1:A:266:VAL:HG12	1.68	0.73
3:D:185:THR:H	3:D:188:HIS:HD2	1.35	0.73
3:D:168:THR:C	3:D:170:PRO:HD2	2.09	0.73
3:D:219:THR:H	3:D:222:HIS:HD2	1.36	0.73
1:A:167:ASP:OD2	1:A:171:ARG:HB3	1.88	0.72
3:D:138:GLU:O	3:D:139:LEU:HD23	1.89	0.72
1:A:76:LEU:HG	1:A:157:VAL:HG21	1.72	0.72
3:D:275:GLU:H	3:D:275:GLU:CD	1.91	0.72
3:D:143:ARG:NH2	3:D:150:LEU:HD21	2.04	0.72
1:A:167:ASP:HB2	1:A:171:ARG:O	1.90	0.72
1:A:291:ASP:CB	1:A:295:ARG:HB2	2.21	0.70
3:D:160:VAL:HG21	3:D:198:ILE:HD12	1.73	0.70
3:D:289:TYR:H	3:D:289:TYR:HD1	1.38	0.70
1:A:297:ARG:HH22	3:D:154:GLN:HG3	1.55	0.70
1:A:50:ARG:HH22	3:D:266:GLN:NE2	1.90	0.69
3:D:125:GLU:O	3:D:128:GLU:HB3	1.91	0.69
2:C:251:VAL:HG13	3:D:249:GLN:CG	2.23	0.68
2:C:251:VAL:HG13	3:D:249:GLN:HG2	1.75	0.68
1:A:168:PRO:HD2	4:A:362:HOH:O	1.93	0.68
2:C:350:GLU:CG	2:C:353:ASP:HB2	2.23	0.68
3:D:165:GLN:OE1	3:D:166:SER:N	2.27	0.68
1:A:171:ARG:HD2	1:A:171:ARG:C	2.14	0.68
1:A:19:PRO:HA	4:A:321:HOH:O	1.94	0.68
1:A:302:ARG:HD3	1:A:302:ARG:H	1.58	0.67
2:C:333:ARG:HH12	2:C:338:GLU:HB2	1.58	0.67
1:A:262:LEU:O	1:A:290:PRO:HB3	1.93	0.67
1:A:301:LYS:HB2	1:A:301:LYS:NZ	2.10	0.66
2:C:252:ARG:HD3	3:D:216:ASN:HB2	1.78	0.65
3:D:119:VAL:CG2	3:D:163:LEU:HD11	2.28	0.64
1:A:158:ARG:HH12	1:A:182:PRO:HD3	1.61	0.64
1:A:118:ILE:HG13	1:A:183:ILE:HD11	1.80	0.64
2:C:272:LYS:HE2	2:C:306:GLN:HG2	1.78	0.64
3:D:188:HIS:O	3:D:192:ILE:HG13	1.98	0.64
1:A:93:LYS:NZ	1:A:93:LYS:HB3	2.13	0.63
1:A:225:GLU:OE2	1:A:275:PRO:HG3	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:185:THR:HG22	3:D:186:CYS:N	2.13	0.63
3:D:219:THR:H	3:D:222:HIS:CD2	2.16	0.63
3:D:245:ARG:HA	3:D:245:ARG:HE	1.61	0.62
3:D:228:GLN:NE2	3:D:262:SER:H	1.97	0.62
1:A:29:GLN:NE2	1:A:222:GLU:HG2	2.14	0.62
1:A:130:ILE:HD12	1:A:131:SER:N	2.15	0.62
3:D:135:CYS:HB3	3:D:139:LEU:HB3	1.81	0.61
3:D:210:ASN:ND2	3:D:242:ASP:H	1.97	0.61
3:D:263:THR:O	3:D:267:GLN:HG3	2.01	0.61
1:A:299:GLU:N	4:A:371:HOH:O	2.33	0.61
2:C:352:LYS:HA	2:C:352:LYS:HZ1	1.65	0.61
3:D:172:LEU:C	3:D:174:SER:H	2.04	0.61
1:A:218:LYS:NZ	1:A:218:LYS:HB3	2.16	0.61
1:A:203:SER:OG	1:A:289:LEU:HD11	2.01	0.61
3:D:243:VAL:HG22	4:D:331:HOH:O	1.99	0.61
3:D:196:LEU:HG	3:D:235:LEU:HD22	1.83	0.60
1:A:41:ARG:HH21	1:A:92:GLY:H	1.46	0.60
2:C:250:ILE:HB	2:C:343:LYS:HE3	1.83	0.60
3:D:201:LEU:O	3:D:201:LEU:HD22	2.01	0.60
3:D:262:SER:OG	3:D:265:ILE:HG13	2.02	0.60
3:D:169:THR:N	3:D:170:PRO:HD2	2.17	0.59
3:D:216:ASN:ND2	3:D:218:ARG:HE	1.99	0.59
2:C:259:CYS:SG	2:C:350:GLU:HB2	2.42	0.59
1:A:33:ARG:CG	1:A:35:ARG:HH12	2.14	0.59
3:D:79:HIS:O	3:D:83:ILE:HG13	2.01	0.59
3:D:258:TRP:HZ3	3:D:278:GLN:O	1.85	0.59
3:D:119:VAL:HG22	3:D:163:LEU:HD11	1.84	0.58
3:D:125:GLU:H	3:D:125:GLU:CD	2.06	0.58
3:D:105:ASN:HB2	3:D:114:PRO:HG2	1.85	0.58
3:D:258:TRP:CZ3	3:D:278:GLN:O	2.57	0.58
3:D:216:ASN:HD22	3:D:218:ARG:NE	2.00	0.57
1:A:265:PRO:HB3	1:A:289:LEU:HD23	1.86	0.57
1:A:110:ILE:N	1:A:110:ILE:HD12	2.20	0.57
1:A:33:ARG:HG3	1:A:35:ARG:NH2	2.18	0.57
1:A:277:ASP:OD1	1:A:279:GLU:HB3	2.05	0.57
1:A:162:GLN:HE22	1:A:174:LEU:HD21	1.70	0.57
3:D:81:ALA:O	3:D:84:HIS:O	2.23	0.57
3:D:129:ALA:O	3:D:131:LEU:HG	2.05	0.57
3:D:229:ASN:O	3:D:233:VAL:HG13	2.04	0.57
1:A:76:LEU:HD13	1:A:90:LEU:HG	1.85	0.57
1:A:297:ARG:HB3	3:D:112:GLN:HE22	1.69	0.56
2:C:324:PRO:CB	2:C:346:LEU:HD11	2.31	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:127:ALA:O	3:D:130:LEU:HD22	2.05	0.56
1:A:194:LEU:HB3	1:A:281:SER:HB3	1.88	0.56
1:A:187:ARG:HH22	1:A:220:GLN:HE22	1.52	0.56
1:A:96:ARG:CZ	1:A:101:GLU:HB3	2.34	0.56
1:A:19:PRO:N	1:A:64:ASN:O	2.39	0.56
1:A:46:ILE:HD11	1:A:118:ILE:HG12	1.87	0.56
3:D:210:ASN:HD21	3:D:242:ASP:N	2.01	0.56
3:D:75:ASP:HA	3:D:79:HIS:ND1	2.20	0.56
2:C:295:PHE:O	2:C:314:PRO:HB3	2.05	0.56
3:D:199:VAL:O	3:D:203:VAL:HG23	2.05	0.55
3:D:172:LEU:HD11	4:D:336:HOH:O	2.06	0.55
1:A:132:GLN:O	1:A:135:GLN:HB2	2.06	0.55
1:A:297:ARG:HB3	3:D:112:GLN:NE2	2.22	0.55
2:C:352:LYS:HA	2:C:352:LYS:HZ2	1.71	0.55
1:A:58:HIS:CD2	1:A:114:GLN:HA	2.41	0.55
1:A:85:PRO:HG3	1:A:139:ASN:HA	1.87	0.55
2:C:334:LYS:HE2	4:C:1:HOH:O	2.06	0.55
2:C:351:ILE:HD12	2:C:352:LYS:N	2.22	0.54
3:D:285:ASP:N	3:D:285:ASP:OD1	2.40	0.54
1:A:219:VAL:HG22	1:A:247:GLN:O	2.06	0.54
2:C:350:GLU:HG2	2:C:353:ASP:HB2	1.88	0.54
1:A:145:ILE:HG21	4:A:309:HOH:O	2.08	0.54
1:A:87:PRO:HB2	1:A:121:VAL:CG1	2.30	0.54
2:C:272:LYS:HD3	2:C:273:VAL:N	2.22	0.54
1:A:112:SER:OG	1:A:114:GLN:NE2	2.41	0.54
1:A:123:LYS:HD2	1:A:126:LEU:HD13	1.90	0.54
1:A:167:ASP:C	1:A:169:ALA:H	2.11	0.53
1:A:196:ILE:CG1	1:A:272:LEU:HD22	2.37	0.53
1:A:236:ARG:HH11	1:A:236:ARG:HG3	1.73	0.53
3:D:135:CYS:HB3	3:D:139:LEU:CB	2.38	0.53
3:D:228:GLN:HE22	3:D:262:SER:H	1.55	0.53
2:C:353:ASP:O	2:C:354:LYS:HB2	2.07	0.53
1:A:57:THR:HG22	1:A:58:HIS:N	2.24	0.53
1:A:239:PHE:HB3	1:A:252:PHE:CB	2.38	0.53
1:A:21:VAL:O	1:A:178:VAL:HG21	2.08	0.53
3:D:144:GLY:O	3:D:180:ASN:HA	2.09	0.53
2:C:278:ILE:HD11	2:C:331:LEU:HB3	1.91	0.53
3:D:135:CYS:O	3:D:139:LEU:HD13	2.08	0.53
1:A:297:ARG:HH22	3:D:154:GLN:CG	2.20	0.53
1:A:198:ARG:NH1	2:C:310:VAL:HG11	2.24	0.53
1:A:246:ARG:HE	3:D:287:GLU:CA	2.22	0.53
2:C:321:ILE:HG13	2:C:323:LYS:H	1.74	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:135:CYS:O	3:D:139:LEU:HB3	2.08	0.52
1:A:251:VAL:HG11	2:C:252:ARG:NH1	2.25	0.52
3:D:244:ASN:O	3:D:245:ARG:O	2.28	0.52
1:A:96:ARG:HH11	1:A:96:ARG:CG	2.23	0.52
1:A:229:THR:CG2	1:A:269:SER:HB3	2.39	0.52
2:C:333:ARG:HH12	2:C:338:GLU:CB	2.23	0.52
1:A:33:ARG:HB3	1:A:186:ASN:ND2	2.25	0.52
3:D:73:ASP:N	4:D:347:HOH:O	2.42	0.52
3:D:136:ASP:N	3:D:137:PRO:CD	2.73	0.52
1:A:41:ARG:NH2	1:A:92:GLY:H	2.08	0.52
1:A:162:GLN:HA	1:A:162:GLN:NE2	2.25	0.52
2:C:284:GLU:O	2:C:291:VAL:HG23	2.10	0.52
3:D:111:GLN:OE1	3:D:142:PHE:HA	2.10	0.52
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.75	0.52
3:D:264:ARG:O	3:D:268:GLN:HG2	2.10	0.51
1:A:196:ILE:HG12	1:A:272:LEU:HD22	1.93	0.51
1:A:218:LYS:HZ3	1:A:218:LYS:HB3	1.75	0.51
1:A:73:ARG:NH2	1:A:138:ASN:OD1	2.43	0.51
1:A:245:HIS:NE2	2:C:307:PHE:HB3	2.25	0.51
1:A:210:ASP:O	1:A:253:ARG:HA	2.10	0.51
3:D:185:THR:HG22	3:D:186:CYS:H	1.73	0.51
1:A:233:TRP:CD1	1:A:258:ALA:HB2	2.46	0.51
3:D:172:LEU:O	3:D:174:SER:N	2.44	0.51
1:A:63:ILE:HD11	1:A:163:VAL:HG11	1.92	0.51
1:A:79:LYS:HA	1:A:158:ARG:CD	2.31	0.51
1:A:246:ARG:HH22	3:D:289:TYR:HB3	1.76	0.51
1:A:162:GLN:CA	1:A:162:GLN:HE21	2.23	0.51
1:A:277:ASP:O	1:A:278:ARG:HB2	2.11	0.51
3:D:181:TYR:C	3:D:182:ASN:HD22	2.14	0.51
2:C:299:SER:OG	2:C:300:PRO:HD2	2.10	0.51
3:D:134:GLY:O	3:D:135:CYS:C	2.49	0.51
3:D:84:HIS:O	3:D:86:GLU:HG2	2.11	0.51
1:A:58:HIS:CG	1:A:114:GLN:HA	2.46	0.51
3:D:101:LEU:O	3:D:102:ALA:HB3	2.10	0.51
3:D:85:GLU:HB3	4:D:345:HOH:O	2.10	0.51
1:A:153:ASP:OD1	1:A:155:ASN:HB2	2.11	0.50
1:A:187:ARG:HH22	1:A:220:GLN:NE2	2.09	0.50
1:A:122:LYS:CD	1:A:122:LYS:N	2.68	0.50
1:A:96:ARG:C	1:A:98:GLY:H	2.14	0.50
1:A:214:LEU:C	1:A:214:LEU:HD23	2.31	0.50
1:A:55:THR:HA	1:A:56:LYS:NZ	2.26	0.50
1:A:86:HIS:CE1	1:A:88:HIS:CD2	2.99	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:138:GLU:O	3:D:140:ARG:NH1	2.44	0.50
3:D:170:PRO:HG2	4:D:305:HOH:O	2.10	0.50
1:A:112:SER:CB	1:A:114:GLN:HE22	2.25	0.50
3:D:94:ILE:HG23	3:D:95:ARG:N	2.26	0.50
2:C:350:GLU:HB3	2:C:353:ASP:HB2	1.93	0.50
1:A:33:ARG:CG	1:A:35:ARG:HH22	2.21	0.50
3:D:143:ARG:HH22	3:D:150:LEU:CD2	2.21	0.49
1:A:227:TYR:CE1	1:A:234:GLU:HG3	2.47	0.49
3:D:137:PRO:CG	3:D:138:GLU:H	2.22	0.49
1:A:217:ASP:OD1	2:C:305:ARG:NH2	2.46	0.49
1:A:28:LYS:CE	1:A:51:SER:HB2	2.43	0.49
1:A:55:THR:HA	1:A:56:LYS:HZ1	1.77	0.49
3:D:113:THR:O	3:D:117:LEU:HD22	2.12	0.49
1:A:89:GLU:HB2	1:A:98:GLY:HA2	1.95	0.49
2:C:313:THR:HG22	2:C:314:PRO:O	2.12	0.49
1:A:202:ASN:HD22	1:A:202:ASN:C	2.16	0.49
1:A:162:GLN:NE2	1:A:174:LEU:HD21	2.27	0.49
2:C:324:PRO:HB2	2:C:346:LEU:CD1	2.39	0.49
1:A:167:ASP:C	1:A:169:ALA:N	2.66	0.49
1:A:32:MET:SD	1:A:46:ILE:HG12	2.54	0.48
2:C:278:ILE:HG13	2:C:279:GLN:N	2.28	0.48
2:C:256:THR:HG21	3:D:214:PRO:HB2	1.95	0.48
1:A:302:ARG:HD3	1:A:302:ARG:N	2.27	0.48
1:A:33:ARG:H	1:A:33:ARG:CZ	2.27	0.48
1:A:94:ASP:HB2	1:A:100:TYR:CE2	2.48	0.48
1:A:246:ARG:HH21	3:D:287:GLU:CB	2.27	0.48
1:A:221:LYS:CE	3:D:280:LEU:HD23	2.44	0.48
1:A:118:ILE:HD12	1:A:157:VAL:HG11	1.95	0.48
3:D:218:ARG:NH1	4:D:361:HOH:O	2.44	0.48
3:D:243:VAL:O	3:D:253:PRO:HD2	2.13	0.48
3:D:282:GLU:HB2	4:D:346:HOH:O	2.13	0.48
3:D:117:LEU:O	3:D:121:THR:HB	2.13	0.47
1:A:229:THR:HG22	1:A:269:SER:HB3	1.95	0.47
1:A:112:SER:HB3	1:A:114:GLN:HE22	1.79	0.47
2:C:251:VAL:O	3:D:248:TYR:HB2	2.15	0.47
1:A:66:TYR:CD1	1:A:67:THR:N	2.82	0.47
1:A:104:LEU:HD22	1:A:111:HIS:CD2	2.50	0.47
3:D:168:THR:N	3:D:170:PRO:HD2	2.29	0.47
1:A:132:GLN:O	1:A:136:THR:HG22	2.14	0.47
2:C:284:GLU:HB2	2:C:327:VAL:HG12	1.95	0.47
3:D:169:THR:N	3:D:170:PRO:CD	2.76	0.47
3:D:135:CYS:SG	3:D:139:LEU:HA	2.55	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:81:PRO:O	1:A:83:HIS:N	2.47	0.47
1:A:33:ARG:O	1:A:35:ARG:NH1	2.47	0.47
1:A:132:GLN:HA	1:A:135:GLN:CG	2.45	0.47
1:A:171:ARG:HD2	1:A:172:PRO:C	2.35	0.47
1:A:129:ALA:O	1:A:133:ARG:HG2	2.15	0.47
1:A:86:HIS:CG	1:A:87:PRO:HD2	2.50	0.47
1:A:233:TRP:HZ3	1:A:268:VAL:HG11	1.79	0.47
2:C:351:ILE:HG12	3:D:111:GLN:HG3	1.97	0.46
1:A:25:GLU:OE2	1:A:57:THR:HG21	2.15	0.46
1:A:301:LYS:HZ2	1:A:301:LYS:HB2	1.80	0.46
3:D:124:PRO:O	3:D:128:GLU:N	2.40	0.46
2:C:352:LYS:HD2	3:D:109:ASN:OD1	2.15	0.46
3:D:172:LEU:HD21	4:D:336:HOH:O	2.15	0.46
1:A:259:ASP:HB3	1:A:262:LEU:HD13	1.98	0.46
1:A:162:GLN:HE22	1:A:174:LEU:CD2	2.28	0.46
1:A:291:ASP:HB2	1:A:295:ARG:NE	2.31	0.45
3:D:279:MET:HG2	3:D:280:LEU:N	2.31	0.45
2:C:321:ILE:HD12	2:C:322:THR:H	1.80	0.45
3:D:119:VAL:HG12	3:D:154:GLN:HE22	1.81	0.45
2:C:350:GLU:CB	2:C:353:ASP:HB2	2.47	0.45
3:D:234:SER:HB3	3:D:268:GLN:HE22	1.81	0.45
1:A:113:PHE:N	1:A:113:PHE:CD1	2.84	0.45
3:D:185:THR:O	3:D:189:LEU:HD22	2.16	0.45
1:A:128:GLN:O	1:A:131:SER:HB3	2.17	0.45
3:D:235:LEU:O	3:D:235:LEU:HG	2.15	0.45
2:C:321:ILE:O	2:C:349:PRO:HB3	2.16	0.45
3:D:230:PRO:HB2	3:D:264:ARG:NE	2.32	0.45
3:D:282:GLU:O	3:D:283:SER:C	2.55	0.45
1:A:221:LYS:O	1:A:241:GLN:HG2	2.17	0.45
1:A:185:ASP:OD1	1:A:186:ASN:N	2.46	0.45
3:D:282:GLU:HG2	3:D:282:GLU:O	2.17	0.45
1:A:300:GLU:N	1:A:300:GLU:OE1	2.50	0.45
3:D:173:HIS:O	3:D:174:SER:O	2.34	0.44
3:D:289:TYR:N	3:D:289:TYR:CD1	2.84	0.44
1:A:28:LYS:HE3	1:A:48:GLY:O	2.17	0.44
1:A:81:PRO:HB2	1:A:82:PRO:CD	2.40	0.44
1:A:126:LEU:O	1:A:130:ILE:HG13	2.17	0.44
1:A:213:PHE:CE2	2:C:252:ARG:HG2	2.52	0.44
3:D:119:VAL:HG12	3:D:154:GLN:NE2	2.32	0.44
3:D:140:ARG:NH1	3:D:146:THR:HG22	2.32	0.44
1:A:127:GLU:O	1:A:130:ILE:HD11	2.17	0.44
1:A:236:ARG:NH1	4:A:334:HOH:O	2.49	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:76:LEU:HG	1:A:157:VAL:CG2	2.45	0.44
1:A:56:LYS:NZ	1:A:56:LYS:H	2.16	0.44
1:A:35:ARG:HB3	1:A:35:ARG:CZ	2.47	0.44
3:D:125:GLU:HA	3:D:128:GLU:HB3	1.99	0.44
2:C:258:GLY:O	2:C:347:TYR:HA	2.17	0.44
1:A:202:ASN:HD22	1:A:202:ASN:H	1.65	0.43
1:A:290:PRO:HB2	1:A:292:THR:HG23	2.00	0.43
3:D:185:THR:N	3:D:188:HIS:HD2	2.09	0.43
2:C:272:LYS:CE	2:C:306:GLN:HG2	2.47	0.43
3:D:275:GLU:CD	3:D:275:GLU:N	2.66	0.43
2:C:268:LEU:C	2:C:268:LEU:HD23	2.38	0.43
1:A:86:HIS:ND1	1:A:87:PRO:HD2	2.34	0.43
1:A:198:ARG:HB3	2:C:267:TYR:OH	2.19	0.43
1:A:59:PRO:O	1:A:113:PHE:HD1	2.01	0.43
1:A:162:GLN:HA	1:A:162:GLN:HE21	1.83	0.43
2:C:323:LYS:HD2	3:D:138:GLU:HG3	2.01	0.43
3:D:86:GLU:HB3	3:D:89:LEU:CB	2.49	0.43
3:D:290:ASP:O	3:D:291:THR:CB	2.66	0.43
3:D:76:SER:C	3:D:78:LEU:H	2.22	0.43
1:A:50:ARG:NH2	3:D:266:GLN:NE2	2.64	0.42
1:A:96:ARG:NH1	1:A:96:ARG:CG	2.81	0.42
1:A:141:PHE:O	1:A:142:HIS:C	2.57	0.42
1:A:37:LYS:HB2	1:A:119:GLN:CD	2.39	0.42
1:A:187:ARG:HH11	1:A:187:ARG:HG2	1.84	0.42
2:C:305:ARG:O	2:C:306:GLN:HB2	2.18	0.42
3:D:201:LEU:O	3:D:204:SER:HB3	2.19	0.42
3:D:177:LYS:HD2	3:D:177:LYS:N	2.34	0.42
3:D:164:THR:HG21	3:D:205:LEU:CD1	2.49	0.42
3:D:113:THR:O	3:D:114:PRO:C	2.58	0.42
3:D:185:THR:CG2	3:D:186:CYS:N	2.82	0.42
3:D:120:ILE:HA	3:D:154:GLN:OE1	2.20	0.42
3:D:133:ALA:HB1	3:D:136:ASP:OD1	2.20	0.42
3:D:198:ILE:O	3:D:202:LEU:HG	2.20	0.42
1:A:93:LYS:HB3	1:A:93:LYS:HZ3	1.82	0.42
1:A:196:ILE:HG13	1:A:272:LEU:HD22	2.01	0.42
2:C:284:GLU:HA	4:C:87:HOH:O	2.18	0.42
1:A:25:GLU:HB3	1:A:60:THR:HB	2.01	0.42
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.82	0.42
1:A:302:ARG:HG3	1:A:302:ARG:HH11	1.84	0.42
3:D:260:ARG:HG3	3:D:260:ARG:HH11	1.84	0.42
3:D:171:HIS:HB2	3:D:174:SER:OG	2.20	0.42
3:D:115:LEU:HD11	3:D:163:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:182:ASN:N	3:D:182:ASN:HD22	2.17	0.42
1:A:202:ASN:ND2	1:A:202:ASN:C	2.73	0.42
2:C:315:LYS:HD2	2:C:315:LYS:N	2.34	0.41
1:A:297:ARG:NH1	3:D:154:GLN:OE1	2.53	0.41
3:D:175:ILE:HG13	3:D:175:ILE:H	1.64	0.41
1:A:36:TYR:CE1	1:A:120:CYS:SG	3.13	0.41
1:A:225:GLU:CD	1:A:275:PRO:HG3	2.41	0.41
3:D:229:ASN:HB3	3:D:232:LEU:HB3	2.02	0.41
1:A:25:GLU:HG2	1:A:58:HIS:O	2.20	0.41
1:A:124:ARG:NH1	1:A:125:ASP:OD2	2.54	0.41
3:D:105:ASN:ND2	3:D:114:PRO:HD2	2.08	0.41
3:D:105:ASN:HB2	3:D:114:PRO:CG	2.50	0.41
1:A:268:VAL:CG1	1:A:269:SER:N	2.82	0.41
3:D:168:THR:HG23	3:D:171:HIS:HD2	1.85	0.41
3:D:222:HIS:CE1	3:D:247:THR:HG23	2.56	0.41
3:D:132:GLY:O	3:D:134:GLY:N	2.54	0.41
1:A:268:VAL:HG12	1:A:269:SER:N	2.36	0.41
1:A:28:LYS:HB3	1:A:47:PRO:HG2	2.03	0.41
1:A:124:ARG:O	1:A:124:ARG:HD3	2.20	0.41
1:A:128:GLN:O	1:A:132:GLN:HG2	2.21	0.41
3:D:196:LEU:HD21	3:D:231:ASP:HB3	2.02	0.41
1:A:30:ARG:NH1	1:A:222:GLU:OE1	2.53	0.41
3:D:224:ALA:CB	3:D:233:VAL:HG12	2.51	0.41
1:A:25:GLU:CD	1:A:57:THR:HG21	2.41	0.41
1:A:57:THR:HG22	1:A:58:HIS:H	1.86	0.41
1:A:74:ILE:HD11	1:A:113:PHE:CE2	2.55	0.41
3:D:148:LEU:HB3	3:D:175:ILE:HG21	2.02	0.41
3:D:172:LEU:O	3:D:173:HIS:HB3	2.21	0.41
2:C:313:THR:HG23	2:C:314:PRO:HD2	2.02	0.41
3:D:140:ARG:HH11	3:D:146:THR:HG22	1.85	0.41
3:D:168:THR:HA	3:D:171:HIS:CD2	2.55	0.41
2:C:251:VAL:CG1	3:D:249:GLN:HG2	2.48	0.41
1:A:214:LEU:O	1:A:249:ALA:HA	2.21	0.41
3:D:78:LEU:O	3:D:82:ILE:N	2.39	0.41
1:A:144:PRO:HG2	1:A:147:GLU:CG	2.51	0.41
3:D:172:LEU:C	3:D:174:SER:N	2.72	0.40
1:A:132:GLN:HA	1:A:135:GLN:HB2	2.04	0.40
1:A:285:GLU:H	1:A:285:GLU:CD	2.25	0.40
1:A:215:LEU:HB3	2:C:304:HIS:CD2	2.56	0.40
1:A:135:GLN:C	1:A:137:ASN:H	2.24	0.40
1:A:34:PHE:HB2	1:A:185:ASP:OD2	2.20	0.40
1:A:262:LEU:HD21	1:A:266:VAL:CG1	2.43	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:TYR:HD2	1:A:122:LYS:NZ	2.20	0.40
1:A:93:LYS:C	1:A:95:CYS:H	2.25	0.40
1:A:56:LYS:H	1:A:56:LYS:CE	2.35	0.40
1:A:35:ARG:HG2	1:A:35:ARG:HH11	1.86	0.40
2:C:332:ARG:HD2	4:C:19:HOH:O	2.19	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	279/286 (98%)	242 (87%)	28 (10%)	9 (3%)	6	3
2	C	111/119 (93%)	101 (91%)	9 (8%)	1 (1%)	25	26
3	D	212/236 (90%)	171 (81%)	26 (12%)	15 (7%)	2	0
All	All	602/641 (94%)	514 (85%)	63 (10%)	25 (4%)	4	2

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	ARG
1	A	292	THR
3	D	135	CYS
3	D	137	PRO
3	D	174	SER
3	D	287	GLU
1	A	42	SER
1	A	43	ALA
1	A	142	HIS
1	A	298	ILE
2	C	355	GLU
3	D	85	GLU
3	D	87	LYS
3	D	133	ALA

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Mol	Chain	Res	Type
3	D	167	CYS
3	D	139	LEU
3	D	245	ARG
3	D	262	SER
3	D	283	SER
3	D	291	THR
1	A	94	ASP
1	A	97	ASP
3	D	175	ILE
3	D	261	PRO
1	A	81	PRO

### 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	251/256 (98%)	228 (91%)	23 (9%)	13	15
2	C	101/108 (94%)	96 (95%)	5 (5%)	34	45
3	D	165/204 (81%)	148 (90%)	17 (10%)	10	11
All	All	517/568 (91%)	472 (91%)	45 (9%)	15	17

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	30	ARG
1	A	33	ARG
1	A	35	ARG
1	A	76	LEU
1	A	81	PRO
1	A	96	ARG
1	A	122	LYS
1	A	132	GLN
1	A	139	ASN
1	A	157	VAL
1	A	162	GLN

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Mol	Chain	Res	Type
1	A	166	ARG
1	A	167	ASP
1	A	183	ILE
1	A	194	LEU
1	A	202	ASN
1	A	271	GLN
1	A	272	LEU
1	A	293	ASP
1	A	294	ASP
1	A	300	GLU
1	A	302	ARG
2	C	286	GLU
2	C	317	LYS
2	C	351	ILE
2	C	352	LYS
2	C	356	GLU
3	D	85	GLU
3	D	104	LEU
3	D	109	ASN
3	D	125	GLU
3	D	135	CYS
3	D	165	GLN
3	D	189	LEU
3	D	227	LEU
3	D	229	ASN
3	D	237	LEU
3	D	245	ARG
3	D	256	LEU
3	D	258	TRP
3	D	275	GLU
3	D	282	GLU
3	D	285	ASP
3	D	289	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	114	GLN
1	A	128	GLN
1	A	162	GLN
1	A	202	ASN

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Mol	Chain	Res	Type
1	A	220	GLN
1	A	271	GLN
3	D	105	ASN
3	D	112	GLN
3	D	171	HIS
3	D	182	ASN
3	D	188	HIS
3	D	210	ASN
3	D	216	ASN
3	D	222	HIS
3	D	228	GLN
3	D	229	ASN
3	D	249	GLN
3	D	266	GLN
3	D	267	GLN
3	D	268	GLN
3	D	271	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	283/286 (98%)	0.82	39 (13%) 4 6	20, 52, 71, 81	0
2	C	113/119 (94%)	0.27	5 (4%) 33 43	20, 39, 69, 77	0
3	D	216/236 (91%)	0.84	30 (13%) 4 6	19, 46, 70, 79	0
All	All	612/641 (95%)	0.73	74 (12%) 5 8	19, 47, 70, 81	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	101	LEU	11.4
1	A	188	ALA	9.5
1	A	298	ILE	9.4
3	D	172	LEU	7.4
3	D	102	ALA	7.3
3	D	106	PHE	6.5
3	D	285	ASP	6.4
2	C	246	SER	6.1
3	D	131	LEU	6.0
3	D	77	PHE	5.9
1	A	54	THR	5.8
1	A	297	ARG	5.2
3	D	95	ARG	5.0
3	D	170	PRO	4.8
1	A	187	ARG	4.6
1	A	292	THR	4.5
3	D	292	GLU	4.3
1	A	191	THR	4.3
2	C	353	ASP	4.2
1	A	40	GLY	4.1
3	D	290	ASP	3.9
1	A	150	GLY	3.9
3	D	293	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	293	ASP	3.8
2	C	352	LYS	3.8
2	C	351	ILE	3.8
1	A	302	ARG	3.7
1	A	294	ASP	3.7
2	C	245	ALA	3.7
1	A	137	ASN	3.6
1	A	145	ILE	3.6
3	D	94	ILE	3.5
1	A	76	LEU	3.5
1	A	42	SER	3.5
1	A	43	ALA	3.3
1	A	124	ARG	3.3
3	D	173	HIS	3.3
1	A	81	PRO	3.2
3	D	139	LEU	3.2
3	D	93	VAL	3.1
3	D	171	HIS	3.1
1	A	134	ILE	3.1
3	D	291	THR	3.1
3	D	137	PRO	3.0
1	A	127	GLU	3.0
1	A	301	LYS	2.9
3	D	282	GLU	2.8
1	A	53	ASP	2.7
1	A	114	GLN	2.6
3	D	105	ASN	2.6
3	D	289	TYR	2.6
3	D	286	GLU	2.5
1	A	299	GLU	2.5
1	A	183	ILE	2.5
1	A	41	ARG	2.5
1	A	242	ALA	2.5
3	D	113	THR	2.4
1	A	86	HIS	2.4
1	A	146	GLU	2.4
1	A	37	LYS	2.4
1	A	300	GLU	2.4
1	A	147	GLU	2.3
3	D	128	GLU	2.3
1	A	128	GLN	2.2
1	A	295	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	135	GLN	2.2
3	D	104	LEU	2.2
1	A	263	GLN	2.2
1	A	39	GLU	2.1
3	D	109	ASN	2.1
3	D	283	SER	2.1
3	D	138	GLU	2.1
1	A	227	TYR	2.0
3	D	103	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.