



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:28 AM GMT

PDB ID : 2QVS  
Title : Crystal Structure of Type IIa Holoenzyme of cAMP-dependent Protein Kinase  
Authors : Wu, J.; Brown, S.H.J.; von Daake, S.; Taylor, S.S.  
Deposited on : 2007-08-08  
Resolution : 2.50 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

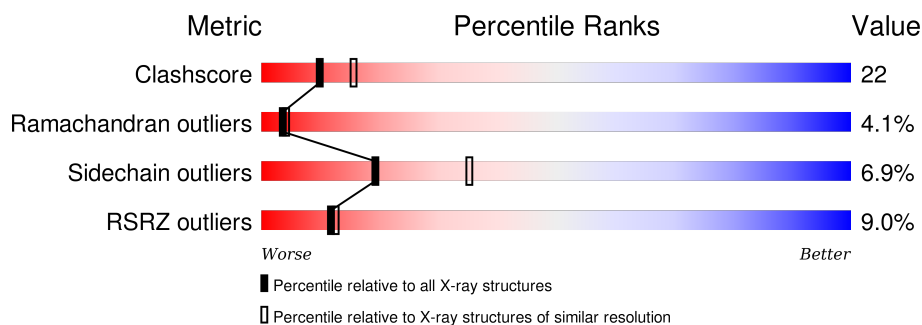
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	E	350	<div> <div>9%</div> <div>58%</div> <div>28%</div> <div>5% • 7%</div> </div>
2	B	310	<div> <div>7%</div> <div>54%</div> <div>38%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5056 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 cAMP-dependent protein kinase, alpha-catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	325	Total	C	N	O	P	S	0	0	0
			2525	1632	430	456	2	5			

- Molecule 2 is a protein called cAMP-dependent protein kinase type II-alpha regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2350	1471	407	457	15			

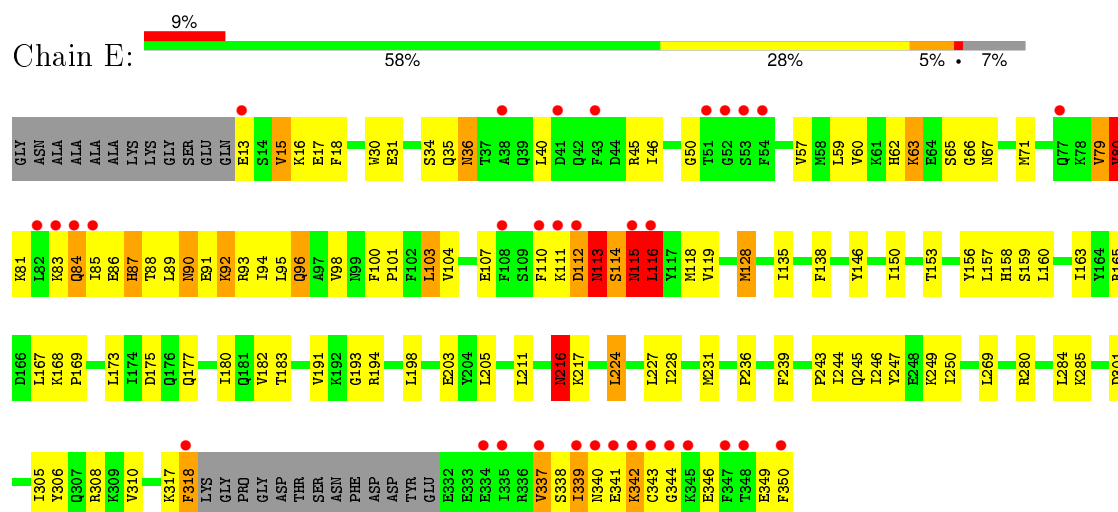
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	75	Total	O	0	0
			75	75		
3	E	106	Total	O	0	0
			106	106		

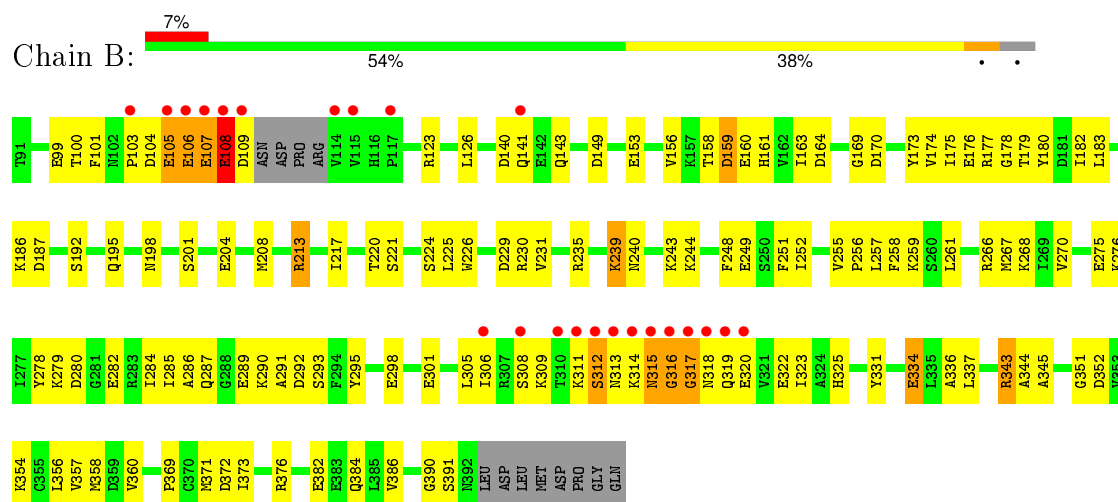
### 3 Residue-property plots

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.

- Molecule 1: cAMP-dependent protein kinase, alpha-catalytic subunit



- Molecule 2: cAMP-dependent protein kinase type II-alpha regulatory subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.90Å 92.90Å 118.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	78.4 (50.00-2.50) 92.0 (48.99-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.212 , 0.251 0.218 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 34006 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5056	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 3.73% 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: TPO, SEP

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	E	0.38	0/2566	0.80	14/3474 (0.4%)
2	B	0.46	0/2383	0.72	5/3203 (0.2%)
All	All	0.42	0/4949	0.76	19/6677 (0.3%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	116	LEU	CA-C-O	11.04	143.29	120.10
1	E	116	LEU	CA-C-N	-10.73	93.58	117.20
1	E	114	SER	CA-C-N	-9.83	95.58	117.20
1	E	81	LYS	N-CA-CB	9.09	126.96	110.60
1	E	114	SER	CA-C-O	9.00	139.01	120.10
1	E	80	VAL	CB-CA-C	-8.97	94.35	111.40
1	E	115	ASN	N-CA-C	8.82	134.81	111.00
1	E	114	SER	CB-CA-C	8.06	125.42	110.10
2	B	314	LYS	N-CA-C	7.66	131.68	111.00
1	E	113	ASN	CB-CA-C	-7.50	95.39	110.40
1	E	114	SER	N-CA-CB	6.68	120.52	110.50
1	E	116	LEU	CB-CA-C	-6.68	97.50	110.20
2	B	314	LYS	CB-CA-C	-6.37	97.66	110.40
1	E	115	ASN	CB-CA-C	-6.24	97.92	110.40
1	E	81	LYS	CA-C-N	-6.14	103.69	117.20
2	B	315	ASN	CA-C-N	-5.33	105.53	116.20
2	B	316	GLY	N-CA-C	5.18	126.05	113.10
2	B	315	ASN	CA-C-O	5.06	130.72	120.10
1	E	81	LYS	CA-C-O	5.05	130.71	120.10

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	E	2525	0	2346	108	0
2	B	2350	0	2301	105	0
3	B	75	0	0	6	0
3	E	106	0	0	4	0
All	All	5056	0	4647	210	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 22.

All (210) 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:108:GLU:N	2:B:108:GLU:OE2	1.95	0.99
1:E:15:VAL:HG23	1:E:16:LYS:HD2	1.46	0.96
2:B:175:ILE:HA	2:B:225:LEU:HD23	1.54	0.88
1:E:285:LYS:HG2	3:E:363:HOH:O	1.74	0.87
2:B:108:GLU:OE2	2:B:108:GLU:CA	2.22	0.86
1:E:59:LEU:HD12	1:E:60:VAL:H	1.42	0.85
1:E:104:VAL:HG11	1:E:183:THR:HG22	1.57	0.84
1:E:16:LYS:H	1:E:16:LYS:HD2	1.48	0.78
2:B:176:GLU:HG3	2:B:177:ARG:HG3	1.68	0.76
1:E:153:THR:O	1:E:157:LEU:HD13	1.85	0.75
2:B:105:GLU:HG2	2:B:105:GLU:O	1.87	0.74
1:E:112:ASP:O	1:E:114:SER:N	2.21	0.74
2:B:305:LEU:O	2:B:345:ALA:HB1	1.88	0.73
1:E:13:GLU:HB2	1:E:15:VAL:HG22	1.70	0.72
1:E:115:ASN:O	1:E:116:LEU:CB	2.40	0.69
1:E:80:VAL:H	1:E:85:ILE:HG21	1.57	0.69
1:E:100:PHE:CD1	1:E:101:PRO:HD2	2.28	0.69
1:E:135:ILE:HD11	1:E:138:PHE:CE1	2.29	0.68
1:E:62:HIS:O	1:E:66:GLY:HA2	1.94	0.68
1:E:113:ASN:HA	1:E:341:GLU:HA	1.74	0.68
2:B:280:ASP:HB2	2:B:351:GLY:HA2	1.75	0.68
1:E:337:VAL:HG23	1:E:339:ILE:H	1.60	0.66
2:B:240:ASN:HB2	3:B:449:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:ASP:C	1:E:114:SER:H	1.99	0.66
1:E:62:HIS:HB3	1:E:67:ASN:H	1.61	0.65
1:E:86:GLU:C	1:E:88:THR:H	2.00	0.65
2:B:140:ASP:OD1	2:B:143:GLN:HG3	1.95	0.65
1:E:40:LEU:HB2	1:E:110:PHE:CE2	2.31	0.65
2:B:235:ARG:NH2	2:B:235:ARG:HB3	2.11	0.65
1:E:35:GLN:HB3	1:E:350:PHE:OXT	1.98	0.64
2:B:182:ILE:HG23	2:B:217:ILE:CD1	2.27	0.64
1:E:80:VAL:H	1:E:85:ILE:CG2	2.10	0.64
2:B:108:GLU:OE2	2:B:108:GLU:HA	1.98	0.63
2:B:311:LYS:O	2:B:312:SER:CB	2.46	0.63
1:E:71:MET:HA	1:E:118:MET:O	1.99	0.62
2:B:291:ALA:HB1	2:B:336:ALA:HB2	1.81	0.62
2:B:331:TYR:CE1	2:B:334:GLU:HG2	2.33	0.62
1:E:146:TYR:HB3	1:E:180:ILE:HD11	1.80	0.62
1:E:128:MET:HE3	1:E:128:MET:HA	1.79	0.62
2:B:256:PRO:HA	2:B:259:LYS:HG2	1.80	0.62
1:E:13:GLU:HB2	1:E:15:VAL:CG2	2.29	0.62
1:E:104:VAL:CG1	1:E:183:THR:HG22	2.28	0.62
2:B:306:ILE:HB	2:B:323:ILE:HD11	1.82	0.62
1:E:100:PHE:CG	1:E:101:PRO:HD2	2.35	0.60
1:E:16:LYS:HD2	1:E:16:LYS:N	2.17	0.60
1:E:193:GLY:HA2	2:B:267:MET:SD	2.42	0.60
2:B:107:GLU:O	2:B:108:GLU:C	2.40	0.60
2:B:235:ARG:HH21	2:B:235:ARG:CB	2.15	0.60
2:B:343:ARG:HH11	2:B:343:ARG:HG3	1.65	0.60
2:B:235:ARG:HH21	2:B:235:ARG:HB3	1.66	0.59
1:E:107:GLU:HB2	1:E:119:VAL:O	2.02	0.59
1:E:342:LYS:O	1:E:344:GLY:N	2.34	0.59
1:E:156:TYR:CD2	1:E:157:LEU:HD12	2.38	0.58
1:E:113:ASN:CA	1:E:341:GLU:HA	2.32	0.58
2:B:101:PHE:HZ	2:B:239:LYS:HZ3	1.50	0.58
2:B:176:GLU:HB3	2:B:224:SER:O	2.04	0.58
2:B:266:ARG:O	2:B:270:VAL:HG23	2.04	0.58
1:E:156:TYR:O	1:E:159:SER:HB3	2.04	0.58
1:E:243:PRO:HA	1:E:246:ILE:HD12	1.85	0.58
1:E:85:ILE:C	1:E:85:ILE:HD12	2.24	0.58
1:E:62:HIS:CD2	1:E:63:LYS:H	2.21	0.58
2:B:275:GLU:OE2	2:B:354:LYS:HE2	2.03	0.58
2:B:278:TYR:CD2	2:B:284:ILE:HG12	2.39	0.58
1:E:150:ILE:HD13	1:E:167:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:LEU:HD23	2:B:174:VAL:HG11	1.86	0.57
2:B:108:GLU:O	2:B:109:ASP:OD1	2.22	0.57
2:B:163:ILE:HB	2:B:213:ARG:HG2	1.86	0.57
1:E:163:ILE:HD12	1:E:165:ARG:HD3	1.85	0.57
1:E:135:ILE:HD11	1:E:138:PHE:HE1	1.69	0.56
2:B:100:THR:HG22	2:B:101:PHE:N	2.21	0.56
1:E:305:ILE:HD12	1:E:310:VAL:HG21	1.87	0.56
2:B:305:LEU:HD23	2:B:322:GLU:HA	1.88	0.56
1:E:107:GLU:HA	1:E:107:GLU:OE1	2.06	0.56
2:B:158:THR:O	2:B:159:ASP:HB2	2.05	0.56
1:E:113:ASN:N	1:E:341:GLU:HG3	2.22	0.56
1:E:89:LEU:HD11	1:E:349:GLU:O	2.05	0.56
1:E:86:GLU:C	1:E:88:THR:N	2.60	0.55
2:B:123:ARG:NH1	2:B:149:ASP:OD2	2.39	0.55
2:B:156:VAL:HG13	2:B:160:GLU:OE1	2.07	0.55
1:E:224:LEU:HD22	1:E:228:ILE:HG13	1.88	0.55
2:B:301:GLU:OE1	2:B:325:HIS:HE1	1.90	0.55
1:E:318:PHE:HD1	1:E:318:PHE:O	1.90	0.55
2:B:251:PHE:O	2:B:255:VAL:HG23	2.07	0.54
1:E:40:LEU:HD12	1:E:40:LEU:O	2.08	0.54
2:B:285:ILE:CG2	2:B:343:ARG:HG2	2.37	0.54
2:B:99:GLU:HG3	2:B:231:VAL:HG22	1.90	0.54
1:E:50:GLY:HA3	1:E:57:VAL:O	2.08	0.53
1:E:342:LYS:C	1:E:344:GLY:H	2.11	0.53
2:B:373:ILE:HA	2:B:376:ARG:HG3	1.89	0.53
1:E:35:GLN:O	1:E:36:ASN:C	2.46	0.53
1:E:18:PHE:HE2	1:E:306:TYR:HH	1.56	0.53
2:B:386:VAL:O	2:B:390:GLY:HA3	2.08	0.53
2:B:276:LYS:HD2	2:B:278:TYR:OH	2.08	0.52
1:E:245:GLN:O	1:E:249:LYS:HG3	2.10	0.52
2:B:293:SER:HB2	2:B:358:MET:O	2.09	0.52
1:E:34:SER:HB3	3:E:389:HOH:O	2.09	0.52
2:B:279:LYS:O	2:B:282:GLU:HG2	2.10	0.52
1:E:15:VAL:HG23	1:E:16:LYS:CD	2.29	0.52
2:B:153:GLU:HB2	2:B:226:TRP:CZ3	2.45	0.51
1:E:227:LEU:O	1:E:231:MET:HG3	2.09	0.51
1:E:59:LEU:HD12	1:E:60:VAL:N	2.18	0.51
2:B:316:GLY:O	2:B:318:ASN:N	2.43	0.51
2:B:182:ILE:C	2:B:183:LEU:HD12	2.30	0.51
2:B:286:ALA:O	2:B:289:GLU:HG2	2.11	0.51
2:B:106:GLU:O	2:B:107:GLU:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:LEU:HD21	1:E:157:LEU:HD11	1.93	0.51
1:E:203:GLU:HG2	1:E:236:PRO:HG3	1.93	0.51
2:B:248:PHE:CE2	2:B:356:LEU:HD21	2.45	0.51
1:E:92:LYS:HD2	1:E:92:LYS:O	2.11	0.50
2:B:169:GLY:HA2	2:B:213:ARG:HH11	1.76	0.50
1:E:246:ILE:O	1:E:250:ILE:HG13	2.12	0.50
1:E:191:VAL:HG13	1:E:216:ASN:HD21	1.76	0.50
1:E:236:PRO:HB2	3:E:364:HOH:O	2.12	0.50
2:B:175:ILE:HG12	2:B:225:LEU:HD21	1.94	0.49
2:B:248:PHE:O	2:B:252:ILE:HG12	2.13	0.49
1:E:135:ILE:HD11	1:E:138:PHE:CD1	2.47	0.49
2:B:235:ARG:O	2:B:239:LYS:HB2	2.12	0.49
1:E:338:SEP:C	1:E:340:ASN:N	2.74	0.49
2:B:107:GLU:O	2:B:109:ASP:OD2	2.30	0.49
1:E:338:SEP:C	1:E:340:ASN:H	2.25	0.49
1:E:111:LYS:CB	1:E:116:LEU:N	2.76	0.49
2:B:244:LYS:HD2	3:B:465:HOH:O	2.13	0.49
2:B:105:GLU:OE1	2:B:243:LYS:HE2	2.13	0.49
2:B:295:TYR:N	2:B:295:TYR:CD2	2.81	0.49
2:B:158:THR:HB	2:B:221:SER:HA	1.94	0.48
1:E:79:VAL:O	1:E:80:VAL:CB	2.61	0.48
1:E:84:GLN:HG3	1:E:85:ILE:N	2.28	0.48
2:B:316:GLY:O	2:B:317:GLY:C	2.51	0.48
1:E:111:LYS:CB	1:E:116:LEU:H	2.26	0.48
2:B:268:LYS:HE3	3:B:463:HOH:O	2.12	0.48
2:B:169:GLY:HA2	2:B:213:ARG:NH1	2.29	0.48
2:B:280:ASP:HB2	2:B:351:GLY:CA	2.42	0.48
2:B:309:LYS:C	2:B:311:LYS:H	2.17	0.48
1:E:112:ASP:C	1:E:114:SER:N	2.65	0.47
2:B:309:LYS:O	2:B:311:LYS:N	2.37	0.47
1:E:84:GLN:HG3	1:E:86:GLU:H	1.79	0.47
1:E:175:ASP:OD2	1:E:308:ARG:NH2	2.45	0.47
2:B:108:GLU:O	2:B:109:ASP:CG	2.53	0.47
2:B:175:ILE:HG12	2:B:225:LEU:CD2	2.44	0.47
1:E:93:ARG:O	1:E:96:GLN:HG3	2.15	0.47
2:B:285:ILE:HG21	2:B:343:ARG:HG2	1.95	0.47
2:B:183:LEU:HD12	2:B:183:LEU:N	2.30	0.47
2:B:105:GLU:CG	2:B:105:GLU:O	2.62	0.47
1:E:104:VAL:HG13	1:E:182:VAL:O	2.15	0.46
2:B:258:PHE:HB3	2:B:261:LEU:HD12	1.97	0.46
1:E:301:ASP:O	1:E:305:ILE:HD13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:HIS:HB3	1:E:217:LYS:HD3	1.96	0.46
1:E:86:GLU:O	1:E:88:THR:N	2.48	0.46
2:B:106:GLU:H	2:B:106:GLU:HG3	1.45	0.46
2:B:343:ARG:HG3	2:B:343:ARG:NH1	2.30	0.46
1:E:317:LYS:NZ	1:E:317:LYS:HB2	2.31	0.46
2:B:278:TYR:HA	2:B:282:GLU:OE2	2.16	0.46
1:E:198:LEU:HD11	2:B:208:MET:HE2	1.98	0.46
2:B:280:ASP:HA	2:B:351:GLY:O	2.15	0.46
1:E:156:TYR:HD2	1:E:157:LEU:HD12	1.80	0.46
2:B:249:GLU:HA	2:B:249:GLU:OE2	2.16	0.46
1:E:35:GLN:HA	1:E:350:PHE:O	2.16	0.45
1:E:191:VAL:HG13	1:E:216:ASN:ND2	2.29	0.45
1:E:177:GLN:NE2	1:E:308:ARG:NH1	2.64	0.45
1:E:244:ILE:HD13	2:B:204:GLU:OE1	2.16	0.45
2:B:293:SER:HA	2:B:360:VAL:HG23	1.98	0.45
2:B:161:HIS:ND1	2:B:164:ASP:OD1	2.46	0.45
1:E:84:GLN:HG3	1:E:85:ILE:H	1.81	0.45
2:B:108:GLU:CD	2:B:108:GLU:H	2.18	0.45
1:E:36:ASN:HA	1:E:110:PHE:HA	1.98	0.45
2:B:298:GLU:HG2	2:B:354:LYS:O	2.17	0.45
2:B:295:TYR:O	2:B:331:TYR:HB2	2.17	0.44
1:E:280:ARG:O	1:E:284:LEU:HD13	2.17	0.44
2:B:178:GLY:N	2:B:198:ASN:OD1	2.50	0.44
1:E:90:ASN:C	1:E:90:ASN:HD22	2.19	0.44
1:E:65:SER:CB	1:E:67:ASN:ND2	2.81	0.44
2:B:276:LYS:HZ3	2:B:357:VAL:HG21	1.81	0.44
2:B:173:TYR:O	2:B:201:SER:HA	2.18	0.44
1:E:128:MET:HG2	1:E:169:PRO:HA	2.00	0.44
1:E:94:ILE:O	1:E:98:VAL:HG22	2.17	0.44
2:B:306:ILE:HG23	2:B:306:ILE:O	2.18	0.43
2:B:287:GLN:HG3	2:B:344:ALA:O	2.18	0.43
1:E:83:LYS:O	1:E:83:LYS:HD3	2.19	0.43
1:E:80:VAL:N	1:E:85:ILE:HG21	2.29	0.43
2:B:292:ASP:O	2:B:360:VAL:HG23	2.18	0.43
2:B:158:THR:HB	2:B:221:SER:CA	2.49	0.43
1:E:167:LEU:O	1:E:168:LYS:HB3	2.18	0.43
2:B:220:THR:HG21	3:B:446:HOH:O	2.19	0.42
2:B:291:ALA:HB3	3:B:404:HOH:O	2.19	0.42
2:B:306:ILE:CB	2:B:323:ILE:HD11	2.48	0.42
1:E:91:GLU:O	1:E:95:LEU:HD23	2.19	0.42
2:B:320:GLU:OE1	2:B:320:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ASN:HD22	1:E:111:LYS:H	1.67	0.42
1:E:193:GLY:O	1:E:194:ARG:NH1	2.49	0.42
1:E:91:GLU:O	1:E:95:LEU:CD2	2.68	0.42
2:B:140:ASP:OD2	2:B:143:GLN:NE2	2.52	0.42
1:E:103:LEU:HD12	1:E:182:VAL:HB	2.01	0.42
1:E:156:TYR:HD2	1:E:157:LEU:CD1	2.33	0.42
1:E:13:GLU:N	1:E:16:LYS:HD3	2.35	0.42
2:B:179:THR:C	2:B:180:TYR:CD1	2.93	0.42
1:E:216:ASN:HB3	3:E:402:HOH:O	2.20	0.42
1:E:203:GLU:OE2	1:E:239:PHE:HA	2.19	0.41
2:B:371:MET:HE3	3:B:456:HOH:O	2.20	0.41
2:B:369:PRO:HG2	2:B:372:ASP:OD2	2.21	0.41
2:B:309:LYS:C	2:B:311:LYS:N	2.73	0.41
1:E:173:LEU:HD13	1:E:183:THR:CG2	2.51	0.41
1:E:205:LEU:HD12	1:E:247:TYR:CE1	2.56	0.41
2:B:103:PRO:HG2	2:B:104:ASP:H	1.85	0.41
2:B:170:ASP:HA	2:B:230:ARG:HH12	1.84	0.41
2:B:337:LEU:HD23	2:B:360:VAL:HG13	2.03	0.40
2:B:186:LYS:O	2:B:187:ASP:HB2	2.20	0.40
2:B:107:GLU:O	2:B:109:ASP:CG	2.60	0.40
2:B:317:GLY:O	2:B:318:ASN:C	2.58	0.40
1:E:317:LYS:CB	1:E:317:LYS:NZ	2.85	0.40
1:E:30:TRP:HZ3	1:E:94:ILE:HG12	1.87	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	E	319/350 (91%)	275 (86%)	28 (9%)	16 (5%)	3	3
2	B	294/310 (95%)	270 (92%)	15 (5%)	9 (3%)	5	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	613/660 (93%)	545 (89%)	43 (7%)	25 (4%)	<b>3</b> <b>4</b>

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	79	VAL
1	E	112	ASP
1	E	115	ASN
1	E	343	CYS
2	B	107	GLU
2	B	308	SER
2	B	312	SER
2	B	315	ASN
2	B	317	GLY
1	E	36	ASN
1	E	80	VAL
1	E	113	ASN
1	E	337	VAL
2	B	391	SER
1	E	46	ILE
1	E	116	LEU
2	B	108	GLU
2	B	313	ASN
2	B	319	GLN
1	E	45	ARG
1	E	63	LYS
1	E	87	HIS
1	E	216	ASN
1	E	346	GLU
1	E	339	ILE

### 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	E	238/303 (78%)	221 (93%)	17 (7%)	<b>18</b> <b>34</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	253/273 (93%)	236 (93%)	17 (7%)	20	37
All	All	491/576 (85%)	457 (93%)	34 (7%)	19	35

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	15	VAL
1	E	17	GLU
1	E	31	GLU
1	E	84	GLN
1	E	87	HIS
1	E	90	ASN
1	E	92	LYS
1	E	96	GLN
1	E	103	LEU
1	E	128	MET
1	E	160	LEU
1	E	211	LEU
1	E	216	ASN
1	E	224	LEU
1	E	269	LEU
1	E	318	PHE
1	E	342	LYS
2	B	105	GLU
2	B	106	GLU
2	B	108	GLU
2	B	141	GLN
2	B	159	ASP
2	B	192	SER
2	B	195	GLN
2	B	213	ARG
2	B	229	ASP
2	B	239	LYS
2	B	257	LEU
2	B	290	LYS
2	B	334	GLU
2	B	343	ARG
2	B	352	ASP
2	B	382	GLU
2	B	384	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such

sidechains are listed below:

Mol	Chain	Res	Type
1	E	35	GLN
1	E	36	ASN
1	E	39	GLN
1	E	62	HIS
1	E	67	ASN
1	E	90	ASN
1	E	96	GLN
1	E	171	ASN
1	E	176	GLN
1	E	177	GLN
1	E	181	GLN
1	E	216	ASN
1	E	289	ASN
1	E	293	ASN
2	B	122	GLN
2	B	127	GLN
2	B	141	GLN
2	B	143	GLN
2	B	146	GLN
2	B	171	ASN
2	B	195	GLN
2	B	325	HIS
2	B	340	ASN
2	B	384	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	E	197	1	8,10,11	0.64	0	7,14,16	1.37	0
1	SEP	E	338	1	8,9,10	0.65	0	8,12,14	1.59	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	E	197	1	-	0/8/11/13	0/0/0/0
1	SEP	E	338	1	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	338	SEP	OG-CB-CA	3.71	111.44	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	338	SEP	2	0

## 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 ⓘ

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	E	323/350 (92%)	0.50	33 (10%) 9 9	21, 42, 100, 101	0
2	B	298/310 (96%)	0.45	23 (7%) 16 18	27, 43, 79, 91	0
All	All	621/660 (94%)	0.47	56 (9%) 12 12	21, 43, 93, 101	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	310	THR	12.1
2	B	315	ASN	9.5
1	E	339	ILE	7.2
2	B	312	SER	6.5
2	B	313	ASN	6.5
1	E	54	PHE	6.4
2	B	106	GLU	6.4
1	E	343	CYS	6.2
2	B	109	ASP	5.7
2	B	319	GLN	5.6
2	B	108	GLU	5.6
1	E	337	VAL	4.8
1	E	51	THR	4.6
1	E	53	SER	4.6
1	E	52	GLY	4.4
2	B	115	VAL	4.4
1	E	340	ASN	4.4
1	E	82	LEU	4.3
2	B	311	LYS	4.3
2	B	105	GLU	4.1
2	B	308	SER	3.7
1	E	345	LYS	3.7
2	B	107	GLU	3.6
1	E	85	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	83	LYS	3.5
2	B	314	LYS	3.4
1	E	350	PHE	3.3
1	E	41	ASP	3.3
2	B	317	GLY	3.1
1	E	318	PHE	3.0
1	E	108	PHE	2.9
1	E	115	ASN	2.9
2	B	114	VAL	2.9
1	E	335	ILE	2.8
1	E	112	ASP	2.8
1	E	334	GLU	2.8
1	E	77	GLN	2.7
1	E	38	ALA	2.6
1	E	110	PHE	2.6
1	E	13	GLU	2.6
1	E	111	LYS	2.5
2	B	103	PRO	2.4
1	E	84	GLN	2.4
1	E	341	GLU	2.4
1	E	43	PHE	2.4
2	B	318	ASN	2.4
2	B	117	PRO	2.3
1	E	347	PHE	2.3
2	B	141	GLN	2.3
2	B	320	GLU	2.2
1	E	348	THR	2.2
1	E	116	LEU	2.2
2	B	316	GLY	2.2
1	E	342	LYS	2.2
1	E	344	GLY	2.1
2	B	306	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	TPO	E	197	11/12	0.98	0.14	-	28,29,30,32	0
1	SEP	E	338	10/11	0.67	0.24	-	100,100,100,100	0

### 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.