



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2017 – 05:47 PM EDT

PDB ID : 3LL8  
Title : Crystal Structure of Calcineurin in Complex with AKAP79 Peptide  
Authors : Li, H.; Hogan, P.G.  
Deposited on : unknown  
Resolution : 2.00 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

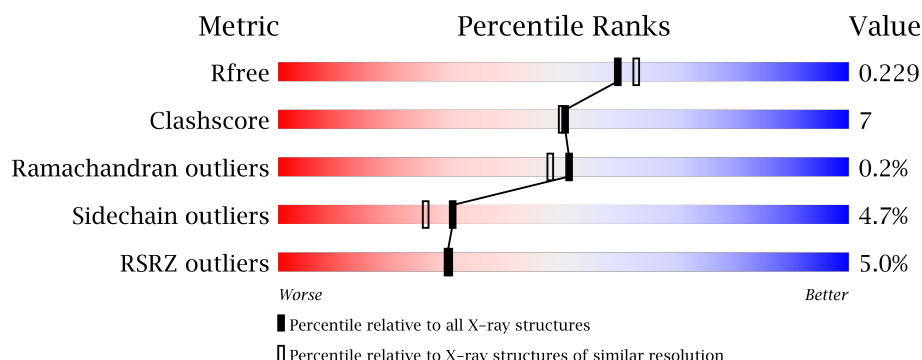
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	11	<div> <div>27%</div> <div>36% 27% 36%</div> </div>
2	A	357	<div> <div>%</div> <div>83% 15% .</div> </div>
2	C	357	<div> <div>2%</div> <div>86% 13% .</div> </div>
3	B	155	<div> <div>14%</div> <div>86% 12% .</div> </div>
3	D	155	<div> <div>11%</div> <div>83% 15% .</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8968 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 AKAP79 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	E	11	Total	C	N	O	0	0	0
			85	54	11	20			

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	357	Total	C	N	O	S	0	0	0
			2903	1870	486	527	20			
2	C	357	Total	C	N	O	S	0	0	0
			2903	1870	486	527	20			

- Molecule 3 is a protein called Calcineurin subunit B type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	155	Total	C	N	O	S	5	0	0
			1236	779	206	245	6			
3	D	155	Total	C	N	O	S	5	0	0
			1236	779	206	245	6			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Fe	0	0
			1	1		
6	C	1	Total	Fe	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	4	Total	Ca	0	0
			4	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	4	Total 4	Ca 4	0	0

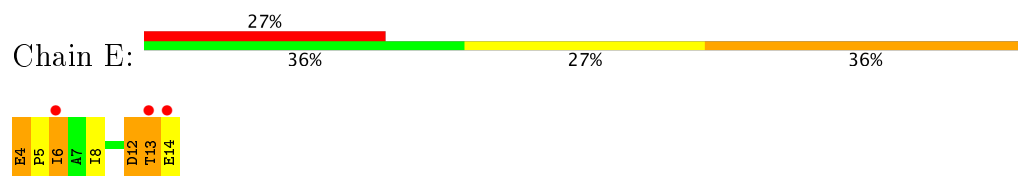
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	5	Total 5	O 5	0	0
8	A	242	Total 242	O 242	0	0
8	B	70	Total 70	O 70	0	0
8	C	228	Total 228	O 228	0	0
8	D	38	Total 38	O 38	0	0

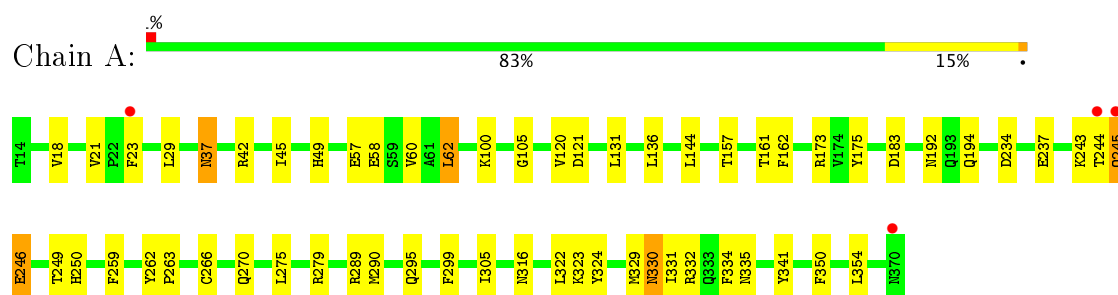
### 3 Residue-property plots [i](#)

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

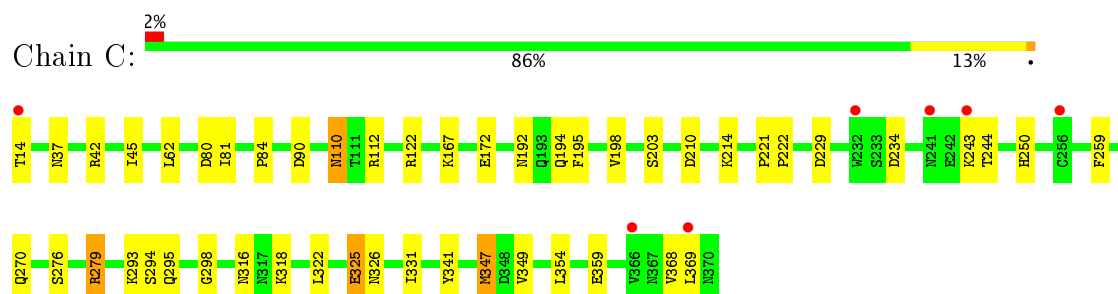
- Molecule 1: AKAP79 peptide



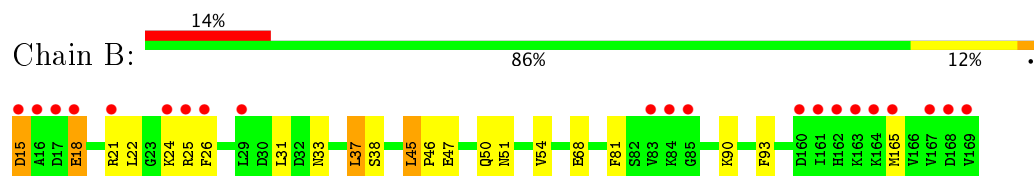
- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform



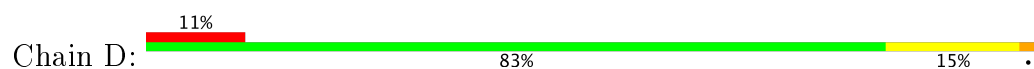
- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

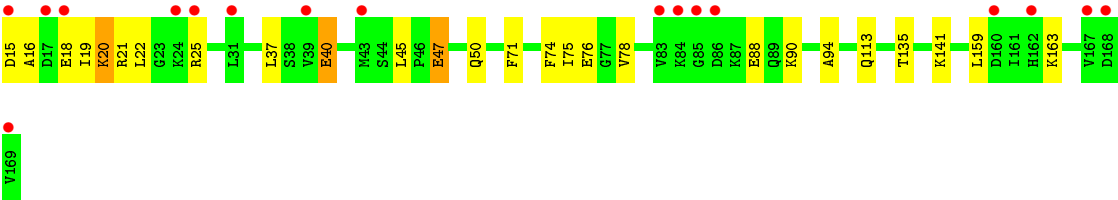


- Molecule 3: Calcineurin subunit B type 1



- Molecule 3: Calcineurin subunit B type 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.28Å 89.70Å 158.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.15 – 2.00 43.16 – 2.01	Depositor EDS
% Data completeness (in resolution range)	95.5 (43.15-2.00) 95.5 (43.16-2.01)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.99 (at 2.00Å)	Xtriage
Refinement program	REFMAC, CNS	Depositor
R, $R_{free}$	0.178 , 0.228 0.178 , 0.229	Depositor DCC
$R_{free}$ test set	3978 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8968	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.95% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN, CA, FE

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	0.89	0/85	0.84	0/115
2	A	0.88	1/2982 (0.0%)	0.82	2/4045 (0.0%)
2	C	0.82	0/2982	0.81	1/4045 (0.0%)
3	B	0.69	0/1251	0.73	0/1672
3	D	0.70	0/1251	0.72	0/1672
All	All	0.81	1/8551 (0.0%)	0.79	3/11549 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	175	TYR	CD1-CE1	5.75	1.48	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	275	LEU	CA-CB-CG	5.81	128.66	115.30
2	C	347	MET	CG-SD-CE	5.42	108.87	100.20
2	A	183	ASP	CB-CG-OD1	5.16	122.94	118.30

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	85	0	85	9	0
2	A	2903	0	2838	39	0
2	C	2903	0	2838	38	0
3	B	1236	0	1225	17	0
3	D	1236	0	1225	18	1
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	B	4	0	0	0	0
7	D	4	0	0	0	0
8	A	242	0	0	7	1
8	B	70	0	0	0	0
8	C	228	0	0	9	2
8	D	38	0	0	1	0
8	E	5	0	0	1	2
All	All	8968	0	8211	110	3

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 7.

All (110) 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)
3:B:15:ASP:HB2	3:B:18:GLU:HB2	1.40	1.04
2:A:341:TYR:OH	2:C:250:HIS:HD2	1.55	0.90
2:A:316:ASN:ND2	8:A:617:HOH:O	2.07	0.86
3:B:15:ASP:CB	3:B:18:GLU:HB2	2.07	0.85
2:C:122:ARG:HD3	8:C:572:HOH:O	1.77	0.84
3:D:113:GLN:HG2	8:D:428:HOH:O	1.80	0.81
2:C:293:LYS:HE2	2:C:298:GLY:O	1.84	0.78
2:C:192:ASN:HD22	2:C:194:GLN:NE2	1.84	0.75
2:A:341:TYR:OH	2:C:250:HIS:CD2	2.42	0.71
1:E:14:GLU:HB2	2:A:335:ASN:HD22	1.55	0.70
2:C:80:ASP:HB3	8:C:485:HOH:O	1.93	0.69
2:A:245:GLN:HB2	8:A:412:HOH:O	1.93	0.67
2:C:84:PRO:HB3	2:C:325:GLU:HG3	1.77	0.67
2:A:332:ARG:NH2	8:A:616:HOH:O	2.28	0.67
2:C:322:LEU:CD1	2:C:331:ILE:HG12	2.25	0.66
2:C:318:LYS:HE3	8:C:475:HOH:O	1.94	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:161:THR:HG23	8:A:450:HOH:O	1.96	0.65
1:E:8:ILE:HD13	2:A:290:MET:SD	2.36	0.65
3:B:15:ASP:N	3:B:15:ASP:OD1	2.30	0.64
2:A:42:ARG:HD3	2:A:45:ILE:HD12	1.79	0.64
2:A:266:CYS:O	2:A:270:GLN:HG2	1.97	0.64
3:B:21:ARG:HA	3:B:24:LYS:HE3	1.81	0.63
3:D:16:ALA:O	3:D:20:LYS:HD2	1.99	0.63
2:C:322:LEU:HD12	2:C:331:ILE:HG12	1.81	0.62
1:E:6:ILE:HD13	2:A:324:TYR:HE1	1.65	0.62
3:B:45:LEU:N	3:B:45:LEU:HD12	2.15	0.62
2:A:250:HIS:HD2	2:C:341:TYR:OH	1.84	0.61
3:D:22:LEU:HD13	3:D:75:ILE:HD12	1.85	0.58
1:E:14:GLU:HB2	2:A:335:ASN:ND2	2.18	0.57
2:A:322:LEU:CD2	2:A:331:ILE:HG12	2.34	0.57
2:C:192:ASN:HB3	2:C:194:GLN:HE21	1.69	0.57
2:C:110:ASN:C	2:C:110:ASN:HD22	2.07	0.57
1:E:13:THR:O	1:E:14:GLU:HG2	2.05	0.57
3:D:71:PHE:CE1	3:D:75:ILE:HD11	2.41	0.55
3:B:26:PHE:CE1	3:B:37:LEU:HD22	2.41	0.54
2:C:326:ASN:O	8:C:567:HOH:O	2.19	0.54
3:D:15:ASP:O	3:D:19:ILE:HG12	2.07	0.54
3:B:15:ASP:HB3	3:B:18:GLU:OE1	2.07	0.54
3:D:47:GLU:N	3:D:47:GLU:OE2	2.36	0.54
1:E:4:GLU:N	1:E:5:PRO:CD	2.71	0.54
2:A:332:ARG:NH1	8:A:504:HOH:O	2.41	0.52
2:A:18:VAL:HG12	2:A:21:VAL:HG23	1.92	0.52
3:B:22:LEU:HD23	3:B:25:ARG:HH11	1.74	0.51
2:A:350:PHE:O	2:A:354:LEU:HB2	2.11	0.51
2:C:42:ARG:HB3	2:C:45:ILE:HD13	1.92	0.51
3:B:90:LYS:HE3	3:B:165:MET:O	2.12	0.50
3:D:15:ASP:HB2	3:D:18:GLU:OE1	2.12	0.50
2:C:167:LYS:HG2	2:C:172:GLU:HG3	1.94	0.50
2:A:249:THR:HG23	8:A:424:HOH:O	2.12	0.49
2:C:322:LEU:HD12	2:C:331:ILE:CG1	2.41	0.49
2:A:192:ASN:HD22	2:A:194:GLN:NE2	2.11	0.49
2:A:234:ASP:O	2:A:259:PHE:HA	2.12	0.49
3:D:15:ASP:OD1	3:D:15:ASP:N	2.45	0.49
2:C:14:THR:N	8:C:571:HOH:O	2.45	0.49
2:C:294:SER:OG	8:C:604:HOH:O	2.19	0.49
3:B:81:PHE:HZ	3:B:93:PHE:CE1	2.31	0.49
1:E:6:ILE:HG12	2:A:299:PHE:CE1	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:234:ASP:O	2:C:259:PHE:HA	2.14	0.48
1:E:4:GLU:N	1:E:5:PRO:HD2	2.28	0.48
2:A:157:THR:HB	2:A:162:PHE:HB3	1.95	0.48
2:A:37:ASN:C	2:A:37:ASN:HD22	2.15	0.48
3:D:74:PHE:O	3:D:78:VAL:HG23	2.14	0.48
2:A:105:GLY:O	2:A:323:LYS:HE3	2.14	0.48
2:A:100:LYS:HE3	2:A:334:PHE:HB2	1.96	0.48
2:C:349:VAL:HG22	3:D:135:THR:HG21	1.96	0.47
3:D:45:LEU:H	3:D:45:LEU:HD12	1.80	0.47
2:C:81:ILE:HG23	2:C:112:ARG:HD3	1.95	0.47
2:C:325:GLU:O	2:C:326:ASN:C	2.54	0.46
2:C:322:LEU:CD1	2:C:331:ILE:CG1	2.94	0.46
2:C:42:ARG:HD3	2:C:45:ILE:HD13	1.97	0.46
3:D:75:ILE:HD13	3:D:75:ILE:N	2.29	0.46
3:D:40:GLU:CD	3:D:40:GLU:H	2.17	0.46
3:B:45:LEU:N	3:B:45:LEU:CD1	2.78	0.46
2:A:57:GLU:HB2	2:A:60:VAL:HG23	1.98	0.46
2:C:122:ARG:NE	8:C:572:HOH:O	2.49	0.46
3:B:45:LEU:CD1	3:B:45:LEU:H	2.29	0.45
2:A:136:LEU:HB3	2:A:144:LEU:HD13	1.98	0.45
3:B:45:LEU:H	3:B:45:LEU:HD12	1.80	0.45
2:A:322:LEU:HD22	2:A:331:ILE:HG12	1.99	0.44
3:B:46:PRO:HD2	3:B:47:GLU:OE2	2.18	0.44
2:C:122:ARG:CD	8:C:572:HOH:O	2.46	0.44
3:B:38:SER:HA	3:B:68:GLU:HG2	1.99	0.44
2:C:368:VAL:HG12	2:C:369:LEU:HD23	2.00	0.44
2:A:131:LEU:HD23	2:A:131:LEU:HA	1.85	0.43
2:C:221:PRO:HA	2:C:222:PRO:HD3	1.81	0.43
3:B:15:ASP:HB3	3:B:18:GLU:CG	2.48	0.43
2:C:195:PHE:HD1	2:C:276:SER:HB3	1.84	0.43
2:A:305:ILE:HD13	2:A:322:LEU:CD2	2.49	0.43
2:A:29:LEU:HG	2:A:49:HIS:CD2	2.54	0.43
2:C:198:VAL:O	2:C:279:ARG:HA	2.19	0.43
3:D:18:GLU:OE1	3:D:18:GLU:N	2.47	0.42
3:D:16:ALA:O	3:D:20:LYS:CD	2.66	0.42
2:A:58:GLU:HG2	2:A:62:LEU:HD22	2.01	0.42
2:C:354:LEU:HD11	3:D:94:ALA:HB1	2.01	0.42
2:C:295:GLN:HA	2:C:295:GLN:NE2	2.35	0.41
1:E:12:ASP:HB2	8:E:403:HOH:O	2.21	0.41
2:A:262:TYR:HB3	2:A:263:PRO:HD3	2.03	0.41
2:A:29:LEU:O	2:A:57:GLU:HG3	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:330:ASN:ND2	2:A:332:ARG:HE	2.18	0.41
3:D:141:LYS:HD2	3:D:141:LYS:HA	1.78	0.41
3:D:21:ARG:HG2	3:D:25:ARG:NH2	2.36	0.41
2:C:214:LYS:HD2	8:C:565:HOH:O	2.19	0.41
2:C:203:SER:HB2	2:C:229:ASP:HB2	2.03	0.41
2:A:250:HIS:CD2	2:C:341:TYR:OH	2.69	0.40
3:B:51:ASN:HB3	3:B:54:VAL:HG23	2.02	0.40
2:A:120:VAL:O	2:A:121:ASP:HB2	2.21	0.40
2:A:244:THR:C	2:A:246:GLU:H	2.24	0.40
2:A:173:ARG:NH2	8:A:581:HOH:O	2.54	0.40
2:C:112:ARG:NH1	2:C:112:ARG:HB2	2.36	0.40
2:C:195:PHE:CD1	2:C:276:SER:HB3	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:403:HOH:O	8:C:531:HOH:O[4_445]	1.94	0.26
8:E:404:HOH:O	8:C:475:HOH:O[4_445]	2.15	0.05
3:D:76:GLU:OE2	8:A:413:HOH:O[3_555]	2.16	0.04

## 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	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
2	A	355/357 (99%)	341 (96%)	13 (4%)	1 (0%)	44	40
2	C	355/357 (99%)	341 (96%)	14 (4%)	0	100	100
3	B	153/155 (99%)	147 (96%)	5 (3%)	1 (1%)	25	18
3	D	153/155 (99%)	148 (97%)	5 (3%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1025/1035 (99%)	985 (96%)	38 (4%)	2 (0%)	51	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	33	ASN
2	A	245	GLN

### 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	10/10 (100%)	6 (60%)	4 (40%)	0	0
2	A	319/319 (100%)	308 (97%)	11 (3%)	42	40
2	C	319/319 (100%)	306 (96%)	13 (4%)	35	31
3	B	138/138 (100%)	132 (96%)	6 (4%)	33	29
3	D	138/138 (100%)	129 (94%)	9 (6%)	20	14
All	All	924/924 (100%)	881 (95%)	43 (5%)	30	26

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	GLU
1	E	6	ILE
1	E	12	ASP
1	E	13	THR
2	A	23	PHE
2	A	37	ASN
2	A	62	LEU
2	A	237	GLU
2	A	243	LYS
2	A	246	GLU
2	A	279	ARG
2	A	289	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	295	GLN
2	A	329	MET
2	A	330	ASN
3	B	15	ASP
3	B	18	GLU
3	B	31	LEU
3	B	37	LEU
3	B	45	LEU
3	B	50	GLN
2	C	37	ASN
2	C	62	LEU
2	C	90	ASP
2	C	110	ASN
2	C	210	ASP
2	C	243	LYS
2	C	244	THR
2	C	270	GLN
2	C	279	ARG
2	C	316	ASN
2	C	325	GLU
2	C	347	MET
2	C	359	GLU
3	D	20	LYS
3	D	37	LEU
3	D	40	GLU
3	D	47	GLU
3	D	50	GLN
3	D	88	GLU
3	D	90	LYS
3	D	159	LEU
3	D	163	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	37	ASN
2	A	194	GLN
2	A	250	HIS
2	A	330	ASN
2	A	335	ASN
2	A	370	ASN
2	C	37	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	110	ASN
2	C	194	GLN
2	C	250	HIS
2	C	295	GLN
2	C	326	ASN
2	C	370	ASN
3	D	50	GLN
3	D	55	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
4	PO4	A	500	5,6	4,4,4	0.76	0	6,6,6	1.21	1 (16%)
4	PO4	C	507	5,6	4,4,4	0.68	0	6,6,6	1.18	0

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
4	PO4	A	500	5,6	-	0/0/0/0	0/0/0/0
4	PO4	C	507	5,6	-	0/0/0/0	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(°)
4	A	500	PO4	O3-P-O1	-2.12	101.93	110.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	E	11/11 (100%)	1.44	3 (27%) 1 1	30, 48, 71, 72	0
2	A	357/357 (100%)	-0.05	4 (1%) 80 80	22, 33, 49, 64	0
2	C	357/357 (100%)	-0.07	7 (1%) 65 65	21, 32, 50, 65	0
3	B	155/155 (100%)	0.41	21 (13%) 3 3	27, 42, 75, 87	2 (1%)
3	D	155/155 (100%)	0.43	17 (10%) 6 6	29, 45, 72, 78	2 (1%)
All	All	1035/1035 (100%)	0.10	52 (5%) 30 30	21, 35, 64, 87	4 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	169	VAL	8.1
3	B	167	VAL	7.7
3	B	168	ASP	6.9
1	E	14	GLU	5.8
3	D	83	VAL	5.7
3	D	168	ASP	5.6
3	D	169	VAL	5.1
3	B	15	ASP	4.8
3	D	84	LYS	4.4
3	B	83	VAL	4.3
1	E	13	THR	4.1
2	A	245	GLN	3.9
2	C	14	THR	3.9
3	B	17	ASP	3.6
3	D	85	GLY	3.5
3	D	167	VAL	3.5
3	B	84	LYS	3.5
2	C	366	VAL	3.4
3	B	162	HIS	3.3
3	B	161	ILE	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	369	LEU	3.0
3	B	165	MET	2.9
3	B	160	ASP	2.9
3	B	25	ARG	2.9
3	D	17	ASP	2.8
3	D	160	ASP	2.8
3	D	31	LEU	2.8
3	B	163	LYS	2.8
2	A	244	THR	2.7
3	B	29	LEU	2.7
3	B	18	GLU	2.6
3	D	86	ASP	2.5
3	B	16	ALA	2.5
3	D	18	GLU	2.4
2	C	232	TRP	2.4
3	B	24	LYS	2.4
2	C	243	LYS	2.4
2	C	256	CYS	2.3
3	B	21	ARG	2.3
3	D	24	LYS	2.3
2	A	23	PHE	2.3
3	D	43	MET	2.3
3	D	15	ASP	2.3
3	D	162	HIS	2.2
3	D	25	ARG	2.2
3	B	26	PHE	2.2
3	D	39	VAL	2.2
2	C	241	ASN	2.2
3	B	85	GLY	2.1
3	B	164	LYS	2.1
1	E	6	ILE	2.0
2	A	370	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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(Å <sup>2</sup> )	Q<0.9
7	CA	B	502	1/1	0.98	0.09	-0.56	32,32,32,32	0
7	CA	B	504	1/1	0.99	0.08	-0.74	35,35,35,35	0
5	ZN	C	512	1/1	1.00	0.13	-1.33	27,27,27,27	0
4	PO4	A	500	5/5	0.99	0.12	-1.35	26,27,29,30	0
7	CA	D	510	1/1	0.99	0.06	-1.54	33,33,33,33	0
7	CA	D	511	1/1	0.99	0.06	-1.79	33,33,33,33	0
5	ZN	A	505	1/1	1.00	0.12	-1.84	27,27,27,27	0
4	PO4	C	507	5/5	0.99	0.08	-2.05	25,26,28,29	0
7	CA	B	501	1/1	0.98	0.05	-2.27	48,48,48,48	0
7	CA	D	509	1/1	0.97	0.04	-2.43	43,43,43,43	0
7	CA	B	503	1/1	1.00	0.05	-2.66	29,29,29,29	0
6	FE	C	513	1/1	0.99	0.06	-2.67	43,43,43,43	0
7	CA	D	508	1/1	0.96	0.03	-2.99	56,56,56,56	0
6	FE	A	506	1/1	0.94	0.07	-3.59	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.