



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:52 PM GMT

PDB ID : 3A3E  
Title : Crystal structure of penicillin binding protein 4 (dacB) from Haemophilus influenzae, complexed with novel beta-lactam (CMV)  
Authors : Kawai, F.; Roper, D.I.; Park, S.-Y.; Tame, J.R.H.  
Deposited on : 2009-06-12  
Resolution : 2.40 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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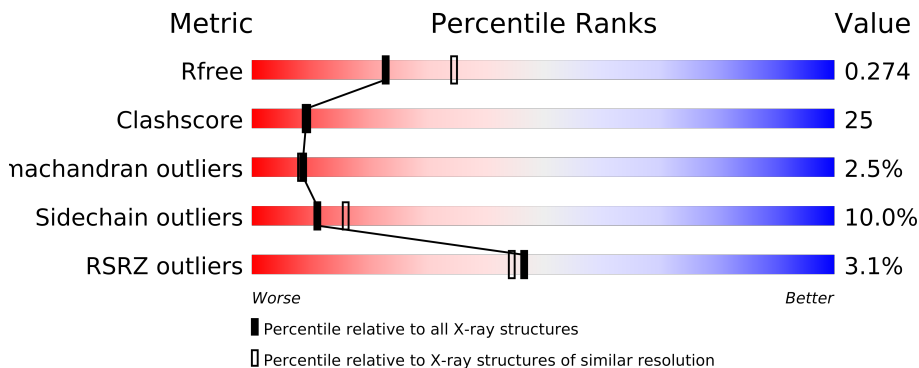
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	453	
1	B	453	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6865 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.

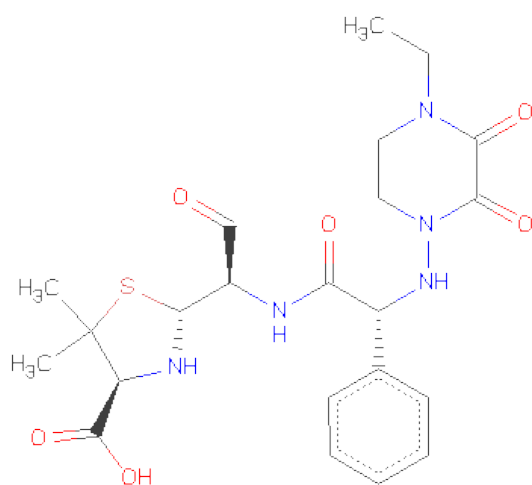
- Molecule 1 is a protein called Penicillin-binding protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3378	2154	582	630	12			
1	B	433	Total	C	N	O	S	0	0	0
			3333	2127	576	620	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	EXPRESSION TAG	UNP A8E0K8
B	27	MET	-	EXPRESSION TAG	UNP A8E0K8

- Molecule 2 is (2R,4S)-2-[(1R)-1-({(2R)-2-[(4-ETHYL-2,3-DIOXOPIPERAZIN-1-YL)AMINO]-2-PHENYLACETYL}AMINO)-2-OXOETHYL]-5,5-DIMETHYL-1,3-THIAZOLIDINE-4-CARBOXYLICACID (three-letter code: CMV) (formula: C<sub>22</sub>H<sub>29</sub>N<sub>5</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	22	5	6	1		
2	B	1	Total	C	N	O	S	0	0
			34	22	5	6	1		

- Molecule 3 is water.

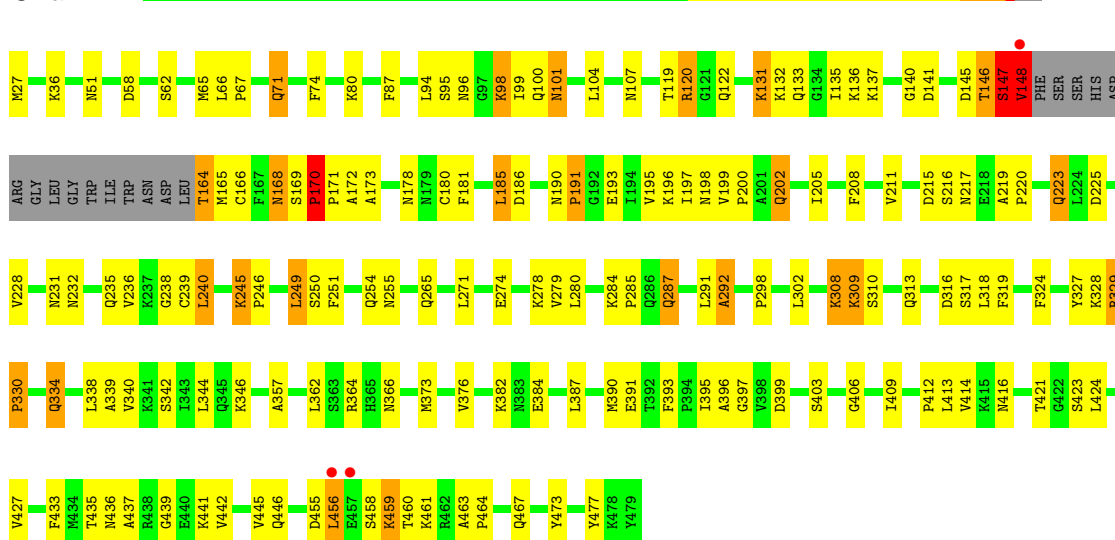
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		
3	B	26	Total	O	0	0
			26	26		

### 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.

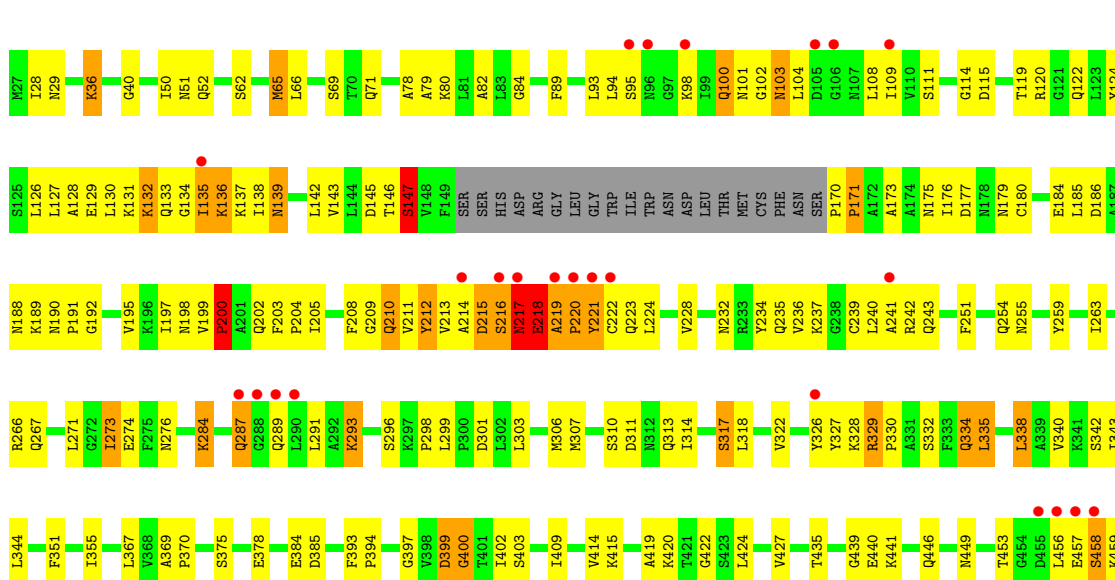
#### • Molecule 1: Penicillin-binding protein 4

Chain A:



#### • Molecule 1: Penicillin-binding protein 4

Chain B:



T460	R461	A463	P464	E469	R470	N471	L472	Y473	L476	Y477	R478	Y479
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.90Å 92.82Å 104.17Å 90.00° 107.79° 90.00°	Depositor
Resolution (Å)	49.57 – 2.40 49.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.57-2.40) 93.0 (49.60-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.217 , 0.280 0.218 , 0.274	Depositor DCC
$R_{free}$ test set	2163 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 30.4	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 42895 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CMV

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	1.05	3/3437 (0.1%)	1.03	3/4644 (0.1%)
1	B	0.93	1/3391 (0.0%)	0.99	6/4582 (0.1%)
All	All	0.99	4/6828 (0.1%)	1.01	9/9226 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	CYS	CB-SG	-7.14	1.70	1.82
1	B	378	GLU	CG-CD	5.59	1.60	1.51
1	A	148	VAL	CB-CG1	5.46	1.64	1.52
1	A	427	VAL	CB-CG1	5.09	1.63	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PRO	C-N-CD	6.83	142.75	128.40
1	A	249	LEU	CA-CB-CG	-6.40	100.58	115.30
1	B	177	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	306	MET	CG-SD-CE	-5.75	91.01	100.20
1	B	456	LEU	CA-CB-CG	5.75	128.51	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	B	399	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	120	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	B	65	MET	CG-SD-CE	5.02	108.23	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	THR	Peptide
1	B	147	SER	Peptide

## 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	3378	0	3440	149	0
1	B	3333	0	3400	193	0
2	A	34	0	26	5	0
2	B	34	0	27	0	0
3	A	60	0	0	3	0
3	B	26	0	0	1	0
All	All	6865	0	6893	341	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 25.

All (341) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:212:TYR:CE2	1:B:239:CYS:HB3	1.66	1.29
1:B:218:GLU:C	1:B:220:PRO:HD2	1.53	1.29
1:B:218:GLU:C	1:B:220:PRO:CD	2.05	1.25
1:A:146:THR:HG22	1:A:147:SER:N	1.45	1.17
1:A:146:THR:CG2	1:A:147:SER:H	1.58	1.17
1:B:215:ASP:O	1:B:217:ASN:N	1.77	1.16

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:124:TYR:CZ	1:B:271:LEU:HD21	1.82	1.13
1:B:137:LYS:HE2	1:B:274:GLU:OE2	1.50	1.10
1:B:219:ALA:N	1:B:220:PRO:HD3	1.61	1.10
1:B:102:GLY:HA3	1:B:136:LYS:HG3	1.39	1.05
1:B:218:GLU:CA	1:B:220:PRO:HD2	1.86	1.05
1:A:357:ALA:H	1:A:366:ASN:ND2	1.54	1.04
1:B:219:ALA:N	1:B:220:PRO:CD	2.17	1.01
1:B:175:ASN:HA	1:B:179:ASN:HD21	1.25	1.01
1:B:191:PRO:HB3	1:B:215:ASP:HA	1.41	1.01
1:A:164:THR:HG22	1:A:165:MET:H	1.22	1.00
1:B:218:GLU:O	1:B:218:GLU:HG2	1.59	1.00
1:B:137:LYS:CE	1:B:274:GLU:OE2	2.09	0.99
1:B:287:GLN:HE21	1:B:287:GLN:HA	1.29	0.98
1:A:80:LYS:HE3	1:A:387:LEU:O	1.64	0.97
1:B:223:GLN:HG2	1:B:224:LEU:H	1.29	0.97
1:B:102:GLY:CA	1:B:136:LYS:HG3	1.94	0.96
1:A:164:THR:CG2	1:A:165:MET:N	2.28	0.96
1:B:212:TYR:CE2	1:B:239:CYS:CB	2.48	0.96
1:A:51:ASN:ND2	1:A:441:LYS:H	1.64	0.96
1:B:209:GLY:C	1:B:210:GLN:HG2	1.83	0.96
1:B:218:GLU:HA	1:B:220:PRO:HD2	1.48	0.95
1:B:397:GLY:HA2	1:B:403:SER:O	1.66	0.95
1:B:124:TYR:OH	1:B:271:LEU:HD23	1.67	0.94
1:A:202:GLN:H	1:A:202:GLN:HE21	1.08	0.93
1:B:129:GLU:O	1:B:133:GLN:HG3	1.68	0.92
1:B:124:TYR:CZ	1:B:271:LEU:CD2	2.52	0.92
1:B:446:GLN:O	1:B:446:GLN:HG2	1.68	0.92
1:B:212:TYR:CD2	1:B:239:CYS:HB3	2.05	0.92
1:B:51:ASN:ND2	1:B:441:LYS:H	1.69	0.91
1:B:232:ASN:HD21	1:B:255:ASN:H	0.96	0.91
1:B:28:ILE:CD1	1:B:476:LEU:HD23	1.99	0.91
1:A:357:ALA:H	1:A:366:ASN:HD21	1.19	0.90
1:A:456:LEU:HD23	1:A:456:LEU:H	1.34	0.90
1:A:164:THR:CG2	1:A:165:MET:H	1.86	0.89
1:B:394:PRO:HG2	1:B:419:ALA:O	1.70	0.89
1:A:99:ILE:CD1	1:A:135:ILE:HD11	2.02	0.88
1:A:228:VAL:HG11	1:A:254:GLN:HG3	1.54	0.88
1:B:212:TYR:HE2	1:B:239:CYS:HB3	1.37	0.88
1:B:460:THR:HG22	1:B:461:LYS:H	1.37	0.87
1:B:461:LYS:HE3	1:B:462:ARG:H	1.39	0.87
1:A:329:ARG:HH12	1:B:221:TYR:HD1	1.23	0.87
1:B:130:LEU:O	1:B:135:ILE:HG13	1.74	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:51:ASN:HD21	1:A:441:LYS:H	1.22	0.87
1:A:329:ARG:NH1	1:B:221:TYR:HD1	1.73	0.86
1:B:191:PRO:HA	1:B:213:VAL:HG12	1.58	0.85
1:B:131:LYS:O	1:B:134:GLY:N	2.07	0.85
1:A:165:MET:HG3	1:A:166:CYS:H	1.41	0.85
1:B:124:TYR:OH	1:B:271:LEU:CD2	2.24	0.85
1:A:71:GLN:HE22	1:A:366:ASN:ND2	1.73	0.85
1:A:232:ASN:HD21	1:A:255:ASN:H	1.25	0.84
1:B:218:GLU:HA	1:B:220:PRO:CD	2.08	0.84
1:B:28:ILE:HD12	1:B:476:LEU:HD23	1.60	0.83
1:B:218:GLU:O	1:B:218:GLU:CG	2.25	0.83
1:B:212:TYR:HE2	1:B:239:CYS:CB	1.88	0.83
1:B:218:GLU:CA	1:B:220:PRO:CD	2.51	0.82
1:A:384:GLU:OE1	1:A:390:MET:HG2	1.80	0.81
1:A:99:ILE:HD11	1:A:135:ILE:HD11	1.60	0.81
1:A:223:GLN:HA	1:A:223:GLN:OE1	1.78	0.81
1:B:232:ASN:HD21	1:B:255:ASN:N	1.76	0.80
1:B:175:ASN:HA	1:B:179:ASN:ND2	1.96	0.80
1:B:232:ASN:ND2	1:B:255:ASN:H	1.76	0.80
1:A:146:THR:CG2	1:A:147:SER:N	2.22	0.80
1:A:131:LYS:HE3	1:A:271:LEU:O	1.81	0.79
1:B:146:THR:HG23	1:B:173:ALA:HB2	1.63	0.79
1:A:36:LYS:HE3	1:A:467:GLN:OE1	1.82	0.79
1:B:287:GLN:NE2	1:B:287:GLN:HA	1.98	0.78
1:B:66:LEU:H	1:B:449:ASN:HD21	1.30	0.78
1:A:148:VAL:HG22	1:A:173:ALA:HB2	1.65	0.78
1:A:329:ARG:O	1:A:330:PRO:C	2.23	0.77
1:B:215:ASP:C	1:B:217:ASN:H	1.87	0.77
1:A:164:THR:HG22	1:A:165:MET:N	1.94	0.77
1:A:95:SER:OG	1:A:104:LEU:HD21	1.84	0.77
1:B:298:PRO:HD2	1:B:301:ASP:OD2	1.86	0.75
1:B:184:GLU:C	1:B:185:LEU:HD12	2.07	0.74
1:B:208:PHE:CZ	1:B:235:GLN:HB2	2.23	0.74
1:B:51:ASN:HD21	1:B:441:LYS:H	1.36	0.74
1:B:131:LYS:O	1:B:133:GLN:N	2.21	0.73
1:B:332:SER:HB2	1:B:334:GLN:OE1	1.89	0.73
1:A:141:ASP:HB3	1:A:278:LYS:O	1.89	0.73
1:A:196:LYS:HE3	1:A:198:ASN:HD21	1.54	0.73
1:B:185:LEU:N	1:B:185:LEU:HD12	2.03	0.73
1:B:334:GLN:H	1:B:334:GLN:CD	1.91	0.72
1:B:241:ALA:O	1:B:243:GLN:HG3	1.90	0.72
1:B:228:VAL:HG21	1:B:254:GLN:HG3	1.72	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:228:VAL:CG1	1:A:254:GLN:HG3	2.20	0.72
1:A:197:ILE:HG13	3:A:11:HOH:O	1.89	0.71
1:B:124:TYR:CE2	1:B:271:LEU:HD21	2.25	0.71
1:B:212:TYR:HE2	1:B:239:CYS:SG	2.14	0.71
1:A:202:GLN:H	1:A:202:GLN:NE2	1.87	0.71
1:B:28:ILE:HD12	1:B:476:LEU:CD2	2.20	0.71
1:A:164:THR:HG23	1:A:165:MET:N	2.04	0.70
1:B:460:THR:CG2	1:B:461:LYS:H	2.03	0.70
1:A:165:MET:CG	1:A:166:CYS:H	2.04	0.70
1:A:287:GLN:OE1	1:A:287:GLN:CA	2.39	0.69
1:B:457:GLU:O	1:B:458:SER:HB3	1.92	0.69
1:B:223:GLN:HG2	1:B:224:LEU:N	2.07	0.69
1:A:202:GLN:HE21	1:A:202:GLN:N	1.87	0.69
1:B:28:ILE:HD11	1:B:476:LEU:HD23	1.75	0.69
1:A:74:PHE:CE1	1:A:376:VAL:HG21	2.27	0.69
1:A:240:LEU:HD12	1:A:240:LEU:N	2.09	0.68
1:B:218:GLU:C	1:B:220:PRO:HD3	1.94	0.68
1:A:240:LEU:HD12	1:A:240:LEU:H	1.59	0.68
1:B:460:THR:HG22	1:B:461:LYS:N	2.09	0.68
1:A:287:GLN:OE1	1:A:287:GLN:HA	1.93	0.67
1:B:216:SER:C	1:B:218:GLU:H	1.98	0.67
1:A:137:LYS:HB2	1:A:274:GLU:HB3	1.75	0.67
1:A:95:SER:CB	1:A:104:LEU:HD21	2.24	0.67
1:A:384:GLU:OE1	1:A:390:MET:CG	2.43	0.67
1:B:104:LEU:O	1:B:139:ASN:HB2	1.94	0.67
1:A:51:ASN:ND2	1:A:441:LYS:N	2.42	0.66
1:A:329:ARG:O	1:A:330:PRO:O	2.13	0.66
1:A:205:ILE:HD12	1:A:205:ILE:C	2.16	0.66
1:B:274:GLU:HG3	1:B:276:ASN:HD21	1.59	0.66
1:A:107:ASN:OD1	1:A:141:ASP:N	2.28	0.66
1:B:130:LEU:HD22	1:B:135:ILE:HD12	1.76	0.66
1:A:170:PRO:O	1:A:172:ALA:N	2.29	0.65
1:A:146:THR:HG22	1:A:147:SER:H	0.65	0.65
1:A:397:GLY:HA2	1:A:403:SER:O	1.97	0.65
1:B:94:LEU:C	1:B:291:LEU:HD12	2.18	0.64
1:B:223:GLN:CG	1:B:224:LEU:H	2.06	0.63
1:B:191:PRO:HB3	1:B:215:ASP:CA	2.23	0.63
1:B:146:THR:HG22	1:B:147:SER:N	2.13	0.63
1:A:357:ALA:N	1:A:366:ASN:HD21	1.94	0.63
1:B:50:ILE:HD12	1:B:441:LYS:HD2	1.81	0.63
1:A:145:ASP:OD1	1:A:146:THR:N	2.32	0.62
1:B:120:ARG:NH1	1:B:202:GLN:O	2.24	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:218:GLU:O	1:B:220:PRO:HD2	1.99	0.61
1:A:74:PHE:HE1	1:A:376:VAL:HG21	1.66	0.61
1:A:329:ARG:NH1	1:B:221:TYR:CD1	2.64	0.61
1:B:469:GLU:O	1:B:473:TYR:HD2	1.84	0.61
1:B:318:LEU:O	1:B:322:VAL:HG23	2.01	0.60
1:A:412:PRO:HG3	1:A:477:TYR:CD2	2.36	0.60
1:A:208:PHE:CE1	1:A:235:GLN:HG3	2.36	0.60
1:B:102:GLY:HA2	1:B:136:LYS:HG3	1.81	0.60
1:B:199:VAL:O	1:B:200:PRO:C	2.39	0.60
1:B:185:LEU:CD1	1:B:185:LEU:N	2.65	0.59
1:B:424:LEU:HD12	1:B:427:VAL:HG21	1.83	0.59
1:A:185:LEU:HD21	1:A:197:ILE:HG23	1.83	0.59
1:B:212:TYR:C	1:B:212:TYR:HD2	2.05	0.59
1:B:394:PRO:HB2	1:B:402:ILE:HG12	1.85	0.59
1:A:327:TYR:O	1:A:329:ARG:HG2	2.03	0.59
1:B:188:ASN:OD1	1:B:242:ARG:NH2	2.35	0.58
1:B:212:TYR:C	1:B:212:TYR:CD2	2.77	0.58
1:B:82:ALA:HB2	1:B:343:ILE:HD13	1.85	0.58
1:B:287:GLN:NE2	1:B:287:GLN:CA	2.66	0.58
1:A:165:MET:CG	1:A:166:CYS:N	2.67	0.58
1:A:169:SER:O	1:A:171:PRO:HD3	2.04	0.57
1:B:215:ASP:C	1:B:217:ASN:N	2.49	0.57
1:A:131:LYS:CE	1:A:271:LEU:O	2.52	0.57
1:B:131:LYS:O	1:B:132:LYS:C	2.40	0.57
1:B:146:THR:HG23	1:B:173:ALA:CB	2.33	0.57
1:A:308:LYS:NZ	1:A:393:PHE:O	2.38	0.56
1:B:89:PHE:N	1:B:296:SER:OG	2.35	0.56
1:B:52:GLN:NE2	1:B:440:GLU:OE2	2.37	0.56
1:B:180:CYS:HB2	1:B:251:PHE:O	2.05	0.56
2:A:1:CMV:HAQ	2:A:1:CMV:OAV	2.04	0.56
2:A:1:CMV:OAT	2:A:1:CMV:CBE	2.54	0.56
1:A:71:GLN:NE2	1:A:366:ASN:ND2	2.51	0.55
1:A:171:PRO:HG3	1:A:316:ASP:HB2	1.89	0.55
1:A:446:GLN:NE2	1:A:473:TYR:OH	2.40	0.54
1:A:186:ASP:O	1:A:195:VAL:HG13	2.06	0.54
1:B:327:TYR:O	1:B:328:LYS:HB2	2.06	0.54
1:B:313:GLN:O	1:B:317:SER:OG	2.26	0.54
1:B:131:LYS:HG3	1:B:273:ILE:HD11	1.89	0.54
1:A:165:MET:HG3	1:A:166:CYS:N	2.17	0.54
1:A:199:VAL:HG12	1:A:200:PRO:O	2.08	0.54
1:B:127:LEU:HD12	1:B:267:GLN:OE1	2.08	0.54
1:B:214:ALA:CB	1:B:240:LEU:O	2.56	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:421:THR:OG1	2:A:1:CMV:O1	2.23	0.53
1:A:456:LEU:H	1:A:456:LEU:CD2	2.08	0.53
1:A:215:ASP:O	1:A:219:ALA:HB2	2.08	0.53
1:A:287:GLN:N	1:A:287:GLN:OE1	2.41	0.53
1:A:216:SER:HA	1:A:219:ALA:CB	2.39	0.53
1:A:302:LEU:HD23	3:A:496:HOH:O	2.09	0.53
1:A:131:LYS:O	1:A:133:GLN:N	2.42	0.53
1:B:95:SER:HB3	1:B:291:LEU:HD11	1.91	0.53
1:B:66:LEU:H	1:B:449:ASN:ND2	2.01	0.52
1:B:146:THR:CG2	1:B:147:SER:N	2.72	0.52
1:B:102:GLY:HA2	1:B:134:GLY:O	2.09	0.52
1:A:382:LYS:HG3	1:A:382:LYS:O	2.08	0.52
1:B:94:LEU:CA	1:B:291:LEU:HD12	2.40	0.52
1:B:214:ALA:O	1:B:216:SER:N	2.35	0.51
1:A:190:ASN:O	1:A:193:GLU:HG3	2.10	0.51
1:A:373:MET:HB3	1:A:445:VAL:HG21	1.92	0.51
1:A:406:GLY:O	1:A:409:ILE:HG13	2.10	0.51
1:A:436:ASN:HA	1:A:477:TYR:HD1	1.76	0.51
1:A:225:ASP:O	1:A:236:VAL:HA	2.11	0.51
1:A:308:LYS:HE3	1:A:399:ASP:OD2	2.11	0.51
1:A:208:PHE:O	1:A:236:VAL:HG12	2.10	0.51
1:A:217:ASN:O	1:A:220:PRO:HD2	2.11	0.51
1:A:329:ARG:C	1:A:330:PRO:O	2.49	0.51
1:A:168:ASN:OD1	1:A:169:SER:N	2.45	0.50
1:B:334:GLN:N	1:B:334:GLN:CD	2.60	0.50
1:A:27:MET:HE1	1:A:58:ASP:HB3	1.94	0.50
1:B:307:MET:CE	1:B:420:LYS:HD3	2.41	0.50
1:A:364:ARG:HD3	3:B:487:HOH:O	2.11	0.50
1:B:188:ASN:O	1:B:189:LYS:HD2	2.11	0.50
1:A:435:THR:HG22	1:A:439:GLY:HA2	1.93	0.50
1:B:114:GLY:O	1:B:115:ASP:C	2.50	0.49
1:B:131:LYS:C	1:B:133:GLN:N	2.63	0.49
1:B:109:ILE:HA	1:B:143:VAL:O	2.13	0.49
1:B:212:TYR:CE2	1:B:239:CYS:SG	2.99	0.49
1:A:413:LEU:O	1:A:416:ASN:HB3	2.12	0.49
1:A:436:ASN:C	1:A:477:TYR:CE1	2.86	0.49
1:A:169:SER:O	1:A:171:PRO:N	2.46	0.49
1:A:169:SER:O	1:A:171:PRO:CD	2.61	0.49
1:A:362:LEU:HD22	2:A:1:CMV:HAU	1.95	0.49
1:B:204:PRO:O	1:B:205:ILE:HD13	2.12	0.49
1:A:190:ASN:O	1:A:191:PRO:C	2.51	0.48
1:B:171:PRO:HG3	1:B:313:GLN:HA	1.93	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:ILE:CD1	1:A:135:ILE:CD1	2.86	0.48
1:B:36:LYS:O	1:B:464:PRO:HB3	2.14	0.48
1:B:274:GLU:HG3	1:B:276:ASN:ND2	2.25	0.48
1:A:74:PHE:CD1	1:A:376:VAL:HG21	2.49	0.48
1:B:216:SER:C	1:B:218:GLU:N	2.65	0.48
1:A:399:ASP:C	1:A:399:ASP:OD1	2.52	0.47
1:A:291:LEU:O	1:A:292:ALA:HB2	2.14	0.47
1:A:145:ASP:OD1	1:A:145:ASP:C	2.52	0.47
1:A:245:LYS:HB3	1:A:246:PRO:CD	2.44	0.47
1:B:228:VAL:HG21	1:B:254:GLN:CG	2.43	0.47
1:B:84:GLY:O	1:B:299:LEU:HD22	2.14	0.47
1:A:100:GLN:O	1:A:101:ASN:C	2.52	0.47
1:A:309:LYS:O	1:A:309:LYS:HG3	2.14	0.47
1:B:80:LYS:HE2	1:B:303:LEU:HD12	1.96	0.47
1:B:209:GLY:O	1:B:210:GLN:HG2	2.12	0.46
1:B:79:ALA:HB1	1:B:299:LEU:HD11	1.96	0.46
1:B:214:ALA:HB3	1:B:240:LEU:O	2.15	0.46
1:B:469:GLU:O	1:B:473:TYR:CD2	2.66	0.46
1:A:245:LYS:HB3	1:A:246:PRO:HD2	1.97	0.46
1:A:357:ALA:N	1:A:366:ASN:ND2	2.39	0.46
1:B:137:LYS:HE3	1:B:274:GLU:OE2	2.07	0.46
1:A:71:GLN:HE22	1:A:366:ASN:HD21	1.60	0.46
1:B:94:LEU:HA	1:B:291:LEU:HD12	1.97	0.46
1:B:211:VAL:HG13	1:B:239:CYS:HA	1.97	0.46
1:B:218:GLU:CA	1:B:220:PRO:HD3	2.37	0.46
1:B:460:THR:CG2	1:B:461:LYS:N	2.72	0.46
1:A:205:ILE:HG22	1:A:232:ASN:HB3	1.98	0.46
1:B:307:MET:HE3	1:B:420:LYS:HD3	1.97	0.46
1:B:214:ALA:C	1:B:216:SER:H	2.16	0.45
1:B:146:THR:CG2	1:B:147:SER:H	2.30	0.45
1:A:265:GLN:NE2	1:A:279:VAL:CG2	2.80	0.45
1:A:412:PRO:CG	1:A:477:TYR:CD2	2.99	0.45
1:B:435:THR:CG2	1:B:439:GLY:HA2	2.46	0.45
1:B:327:TYR:OH	1:B:338:LEU:HB3	2.17	0.45
1:A:216:SER:HA	1:A:219:ALA:HB3	1.99	0.45
1:A:98:LYS:HE3	1:A:98:LYS:HB3	1.51	0.45
1:A:328:LYS:C	1:A:329:ARG:HG2	2.37	0.45
1:A:436:ASN:HA	1:A:477:TYR:CD1	2.51	0.45
1:A:395:ILE:O	1:A:396:ALA:C	2.55	0.45
1:B:311:ASP:OD1	1:B:314:ILE:HG13	2.17	0.44
1:A:66:LEU:HA	1:A:67:PRO:HD2	1.83	0.44
1:B:145:ASP:C	1:B:145:ASP:OD1	2.56	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:414:VAL:CG1	1:B:414:VAL:O	2.65	0.44
1:B:186:ASP:O	1:B:195:VAL:HG13	2.17	0.44
1:A:87:PHE:O	1:A:298:PRO:HA	2.17	0.44
1:B:65:MET:HB3	1:B:449:ASN:ND2	2.31	0.44
1:B:51:ASN:ND2	1:B:441:LYS:N	2.51	0.44
1:A:245:LYS:CD	1:A:245:LYS:N	2.80	0.44
1:B:80:LYS:HE2	1:B:303:LEU:CD1	2.47	0.44
1:B:203:PHE:HB3	1:B:205:ILE:HG12	1.99	0.44
1:A:231:ASN:CG	1:A:231:ASN:O	2.56	0.44
1:A:95:SER:HB2	1:A:104:LEU:HD21	2.00	0.44
1:A:169:SER:O	1:A:170:PRO:C	2.56	0.44
1:A:65:MET:O	1:A:67:PRO:HD3	2.18	0.43
1:B:293:LYS:HE3	1:B:293:LYS:HB2	1.65	0.43
1:A:181:PHE:CZ	1:A:251:PHE:HB2	2.53	0.43
1:B:211:VAL:HG11	1:B:224:LEU:HD11	2.01	0.43
1:B:414:VAL:HG13	1:B:414:VAL:O	2.19	0.43
1:B:314:ILE:HG22	1:B:318:LEU:HD12	2.00	0.43
1:B:384:GLU:O	1:B:385:ASP:C	2.56	0.43
1:B:284:LYS:HB3	1:B:284:LYS:HE2	1.58	0.43
1:A:107:ASN:OD1	1:A:140:GLY:HA3	2.19	0.43
1:A:436:ASN:OD1	1:A:436:ASN:C	2.56	0.43
1:B:69:SER:HB2	1:B:422:GLY:HA2	2.00	0.43
1:B:66:LEU:N	1:B:449:ASN:HD21	2.06	0.43
1:A:463:ALA:N	1:A:464:PRO:CD	2.82	0.43
1:B:170:PRO:HA	1:B:171:PRO:HD3	1.64	0.43
1:B:414:VAL:O	1:B:415:LYS:HB2	2.19	0.43
1:A:62:SER:O	1:B:40:GLY:HA2	2.19	0.43
1:A:446:GLN:HG2	1:A:446:GLN:O	2.19	0.42
1:B:93:LEU:HD11	1:B:126:LEU:O	2.18	0.42
1:A:249:LEU:HA	1:A:249:LEU:HD23	1.63	0.42
1:B:259:TYR:CE2	1:B:263:ILE:HD11	2.54	0.42
1:A:120:ARG:NH1	1:A:202:GLN:O	2.40	0.42
1:B:127:LEU:O	1:B:130:LEU:HB2	2.19	0.42
1:A:216:SER:O	1:A:220:PRO:HD3	2.18	0.42
1:B:100:GLN:HB3	1:B:101:ASN:H	1.61	0.42
1:A:232:ASN:ND2	1:A:255:ASN:H	2.05	0.42
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.92	0.42
1:B:84:GLY:O	1:B:299:LEU:CD2	2.67	0.42
1:A:319:PHE:CE1	1:A:340:VAL:HG21	2.54	0.42
1:B:104:LEU:HD23	1:B:138:ILE:HG23	2.01	0.42
1:B:344:LEU:HD12	1:B:351:PHE:HZ	1.84	0.42
1:A:324:PHE:O	1:A:328:LYS:HA	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:108:LEU:O	1:B:142:LEU:HD12	2.20	0.42
1:B:222:CYS:SG	1:B:239:CYS:C	2.98	0.42
1:B:28:ILE:HG22	1:B:29:ASN:N	2.34	0.42
1:A:346:LYS:HE2	1:A:346:LYS:HB3	1.60	0.42
1:A:433:PHE:HA	1:A:442:VAL:O	2.20	0.42
1:A:216:SER:HA	1:A:219:ALA:HB2	2.00	0.42
1:B:274:GLU:O	1:B:274:GLU:HG2	2.20	0.42
1:B:36:LYS:HE3	1:B:471:ASN:HD22	1.84	0.41
1:B:234:TYR:CD2	1:B:234:TYR:N	2.88	0.41
1:B:393:PHE:HA	1:B:394:PRO:HD2	1.87	0.41
1:B:146:THR:HG22	1:B:147:SER:H	1.84	0.41
1:B:185:LEU:HG	1:B:197:ILE:HG12	2.02	0.41
1:B:223:GLN:CG	1:B:224:LEU:N	2.78	0.41
1:B:176:ILE:H	1:B:179:ASN:ND2	2.19	0.41
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.90	0.41
1:B:355:ILE:N	1:B:367:LEU:O	2.47	0.41
1:B:211:VAL:HG23	1:B:236:VAL:HG23	2.02	0.41
1:A:437:ALA:HA	1:A:477:TYR:CE1	2.55	0.41
1:A:459:LYS:H	1:A:459:LYS:HG3	1.52	0.41
1:B:119:THR:OG1	1:B:122:GLN:HG3	2.21	0.41
1:A:423:SER:O	1:A:424:LEU:HD23	2.20	0.41
1:B:78:ALA:HB2	1:B:340:VAL:HG13	2.03	0.41
1:B:399:ASP:O	1:B:400:GLY:O	2.39	0.41
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.86	0.41
1:B:222:CYS:SG	1:B:239:CYS:O	2.78	0.41
1:B:28:ILE:CG2	1:B:29:ASN:N	2.82	0.41
1:B:335:LEU:HD13	1:B:335:LEU:HA	1.90	0.41
1:A:285:PRO:HB3	3:A:7:HOH:O	2.20	0.41
1:B:369:ALA:O	1:B:370:PRO:C	2.59	0.41
1:A:178:ASN:HA	1:A:313:GLN:HE22	1.85	0.41
1:A:119:THR:OG1	1:A:122:GLN:HG3	2.20	0.41
1:B:101:ASN:C	1:B:103:ASN:H	2.25	0.40
1:A:334:GLN:H	1:A:334:GLN:CD	2.20	0.40
1:B:338:LEU:HA	1:B:338:LEU:HD12	1.89	0.40
1:A:211:VAL:HA	1:A:238:GLY:O	2.21	0.40
1:B:184:GLU:OE1	1:B:198:ASN:HB2	2.22	0.40
1:A:185:LEU:CD2	1:A:197:ILE:HG23	2.49	0.40
1:A:327:TYR:CE2	1:A:339:ALA:HB2	2.57	0.40
1:B:128:ALA:C	1:B:130:LEU:N	2.74	0.40
2:A:1:CMV:OAT	2:A:1:CMV:HBEA	2.21	0.40
1:B:329:ARG:HB2	1:B:330:PRO:HD2	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	434/453 (96%)	406 (94%)	20 (5%)	8 (2%)	13	15
1	B	429/453 (95%)	384 (90%)	31 (7%)	14 (3%)	6	5
All	All	863/906 (95%)	790 (92%)	51 (6%)	22 (2%)	9	8

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	B	171	PRO
1	B	215	ASP
1	B	216	SER
1	B	218	GLU
1	B	219	ALA
1	B	220	PRO
1	A	101	ASN
1	A	132	LYS
1	B	132	LYS
1	B	217	ASN
1	B	400	GLY
1	B	458	SER
1	B	147	SER
1	B	221	TYR
1	A	131	LYS
1	A	330	PRO
1	A	170	PRO
1	A	292	ALA
1	A	191	PRO
1	B	200	PRO
1	B	192	GLY

### 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	365/378 (97%)	329 (90%)	36 (10%)	11	16
1	B	358/378 (95%)	322 (90%)	36 (10%)	11	16
All	All	723/756 (96%)	651 (90%)	72 (10%)	11	16

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	94	LEU
1	A	96	ASN
1	A	98	LYS
1	A	136	LYS
1	A	147	SER
1	A	148	VAL
1	A	164	THR
1	A	168	ASN
1	A	185	LEU
1	A	202	GLN
1	A	223	GLN
1	A	239	CYS
1	A	240	LEU
1	A	245	LYS
1	A	250	SER
1	A	280	LEU
1	A	284	LYS
1	A	287	GLN
1	A	308	LYS
1	A	309	LYS
1	A	310	SER
1	A	317	SER
1	A	318	LEU
1	A	329	ARG
1	A	334	GLN
1	A	338	LEU
1	A	342	SER
1	A	391	GLU

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Mol	Chain	Res	Type
1	A	414	VAL
1	A	455	ASP
1	A	456	LEU
1	A	458	SER
1	A	459	LYS
1	A	460	THR
1	A	461	LYS
1	B	36	LYS
1	B	62	SER
1	B	71	GLN
1	B	98	LYS
1	B	100	GLN
1	B	103	ASN
1	B	111	SER
1	B	135	ILE
1	B	136	LYS
1	B	139	ASN
1	B	190	ASN
1	B	200	PRO
1	B	210	GLN
1	B	212	TYR
1	B	217	ASN
1	B	218	GLU
1	B	237	LYS
1	B	273	ILE
1	B	284	LYS
1	B	287	GLN
1	B	289	GLN
1	B	293	LYS
1	B	310	SER
1	B	317	SER
1	B	326	TYR
1	B	329	ARG
1	B	334	GLN
1	B	335	LEU
1	B	338	LEU
1	B	342	SER
1	B	375	SER
1	B	409	ILE
1	B	453	THR
1	B	459	LYS
1	B	461	LYS

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Mol	Chain	Res	Type
1	B	478	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	51	ASN
1	A	101	ASN
1	A	178	ASN
1	A	198	ASN
1	A	202	GLN
1	A	206	GLN
1	A	232	ASN
1	A	235	GLN
1	A	243	GLN
1	A	265	GLN
1	A	313	GLN
1	A	366	ASN
1	A	446	GLN
1	B	51	ASN
1	B	71	GLN
1	B	103	ASN
1	B	179	ASN
1	B	217	ASN
1	B	232	ASN
1	B	235	GLN
1	B	276	ASN
1	B	283	GLN
1	B	286	GLN
1	B	287	GLN
1	B	383	ASN
1	B	449	ASN
1	B	471	ASN

### 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 ⓘ

2 ligands 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$
2	CMV	A	1	1	36,36,36	3.65	8 (22%)	52,52,52	5.69	25 (48%)
2	CMV	B	1	1	36,36,36	3.55	8 (22%)	52,52,52	3.36	24 (46%)

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
2	CMV	A	1	1	-	3/23/60/60	0/3/3/3
2	CMV	B	1	1	-	2/23/60/60	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	CMV	NAN-NAG	-14.72	1.23	1.41
2	B	1	CMV	NAN-NAG	-14.27	1.23	1.41
2	B	1	CMV	CAE-CAI	-11.39	1.31	1.53
2	A	1	CMV	CAE-CAI	-9.02	1.36	1.53
2	A	1	CMV	CAE-NAG	-8.18	1.30	1.37
2	B	1	CMV	C6-S1	-7.15	1.70	1.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	CMV	C6-S1	-6.68	1.71	1.85
2	A	1	CMV	CAW-CAM	-4.90	1.44	1.52
2	A	1	CMV	C13-S1	-4.59	1.71	1.85
2	B	1	CMV	C13-S1	-3.96	1.73	1.85
2	B	1	CMV	C14-C15	3.41	1.53	1.50
2	B	1	CMV	C14-N1	3.03	1.49	1.46
2	A	1	CMV	CAM-CAL	-2.44	1.48	1.53
2	B	1	CMV	C12-C2	-2.43	1.49	1.52
2	B	1	CMV	CAW-CAM	-2.10	1.49	1.52
2	A	1	CMV	C13-C14	2.09	1.59	1.54

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	CMV	CAQ-NAG-NAN	28.56	130.43	109.56
2	A	1	CMV	CAM-NAN-NAG	19.96	136.08	112.56
2	B	1	CMV	CAM-NAN-NAG	13.52	128.49	112.56
2	A	1	CMV	CAE-NAG-NAN	-10.04	104.20	118.08
2	B	1	CMV	CAQ-NAG-NAN	9.77	116.70	109.56
2	A	1	CMV	OAS-CAE-NAG	-7.99	112.50	120.74
2	B	1	CMV	CAQ-NAG-CAE	6.09	129.68	120.91
2	B	1	CMV	OAS-CAE-NAG	5.91	126.83	120.74
2	A	1	CMV	CAL-CAM-NAN	5.39	123.69	108.19
2	B	1	CMV	C14-C13-N3	-5.35	100.98	112.69
2	A	1	CMV	C1-C6-S1	5.33	118.19	109.15
2	A	1	CMV	CBB-NAO-CAI	4.97	125.68	119.69
2	A	1	CMV	CAU-CAQ-NAG	-4.85	104.62	111.76
2	A	1	CMV	OAS-CAE-CAI	4.44	128.99	118.69
2	A	1	CMV	CBD-CAW-CBC	4.26	123.98	118.33
2	B	1	CMV	OAT-CAI-NAO	4.14	128.19	123.58
2	A	1	CMV	C16-C6-C1	-4.08	104.04	110.90
2	A	1	CMV	C14-C13-S1	3.97	121.43	110.25
2	A	1	CMV	C6-S1-C13	3.70	101.99	94.01
2	B	1	CMV	CAL-CAM-NAN	-3.53	98.04	108.19
2	B	1	CMV	CBB-NAO-CAI	3.48	123.88	119.69
2	B	1	CMV	C6-C12-C2	3.38	117.29	112.55
2	B	1	CMV	CAW-CAM-CAL	3.34	115.17	107.77
2	B	1	CMV	C6-S1-C13	3.32	101.16	94.01
2	B	1	CMV	CAE-CAI-NAO	-3.27	115.82	117.41
2	B	1	CMV	S1-C13-N3	-3.27	102.25	106.66
2	B	1	CMV	CAE-NAG-NAN	-3.23	113.62	118.08
2	A	1	CMV	CAW-CAM-NAN	-3.22	102.62	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	CMV	CAM-CAL-N1	3.04	125.36	116.92
2	B	1	CMV	C14-N1-CAL	-3.02	118.02	123.09
2	B	1	CMV	OAV-CAL-CAM	-2.99	115.37	120.52
2	A	1	CMV	CAQ-NAG-CAE	2.98	125.20	120.91
2	B	1	CMV	C14-C13-S1	2.96	118.59	110.25
2	A	1	CMV	CBC-CAW-CAM	-2.83	115.87	120.82
2	A	1	CMV	C14-C13-N3	-2.81	106.53	112.69
2	B	1	CMV	C16-C6-S1	2.80	113.91	109.15
2	A	1	CMV	S1-C13-N3	-2.78	102.91	106.66
2	A	1	CMV	CBG-CBD-CAW	-2.73	117.00	120.61
2	A	1	CMV	CAW-CAM-CAL	2.73	113.82	107.77
2	A	1	CMV	CAU-NAO-CBB	-2.70	111.02	116.20
2	B	1	CMV	C16-C6-C1	-2.70	106.36	110.90
2	B	1	CMV	C2-C12-N3	-2.57	106.13	110.67
2	A	1	CMV	O1-C2-C12	2.53	122.45	113.19
2	A	1	CMV	C13-C14-C15	-2.41	108.29	112.03
2	B	1	CMV	CAU-CAQ-NAG	-2.40	108.22	111.76
2	A	1	CMV	C13-N3-C12	2.25	114.99	109.62
2	A	1	CMV	C1-C6-C12	-2.25	106.87	112.05
2	B	1	CMV	C6-C12-N3	-2.09	104.93	108.52
2	B	1	CMV	C13-C14-C15	-2.07	108.81	112.03

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	CMV	CAM-NAN-NAG-CAQ
2	A	1	CMV	CAM-NAN-NAG-CAQ
2	A	1	CMV	CBE-CBB-NAO-CAI
2	B	1	CMV	CAM-NAN-NAG-CAE
2	A	1	CMV	CAM-NAN-NAG-CAE

There are no ring outliers.

## 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	438/453 (96%)	-0.00	3 (0%) 84 84	16, 32, 54, 76	0
1	B	433/453 (95%)	0.27	24 (5%) 24 22	18, 40, 72, 86	0
All	All	871/906 (96%)	0.14	27 (3%) 47 44	16, 36, 67, 86	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	456	LEU	6.8
1	B	217	ASN	4.7
1	B	220	PRO	4.7
1	B	457	GLU	4.2
1	B	221	TYR	4.2
1	B	96	ASN	4.0
1	B	287	GLN	3.9
1	B	219	ALA	3.5
1	B	222	CYS	3.5
1	B	98	LYS	3.3
1	B	326	TYR	3.1
1	B	216	SER	2.9
1	B	135	ILE	2.9
1	A	456	LEU	2.8
1	B	214	ALA	2.8
1	B	289	GLN	2.7
1	B	95	SER	2.7
1	A	148	VAL	2.6
1	B	288	GLY	2.5
1	B	458	SER	2.4
1	B	241	ALA	2.4
1	B	109	ILE	2.3
1	B	105	ASP	2.2
1	A	457	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	106	GLY	2.1
1	B	290	LEU	2.1
1	B	455	ASP	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 ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CMV	B	1	34/34	0.13	-0.58	25,33,54,57	0
2	CMV	A	1	34/34	0.14	-0.86	15,25,46,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.