Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 03:55 PM EDT

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

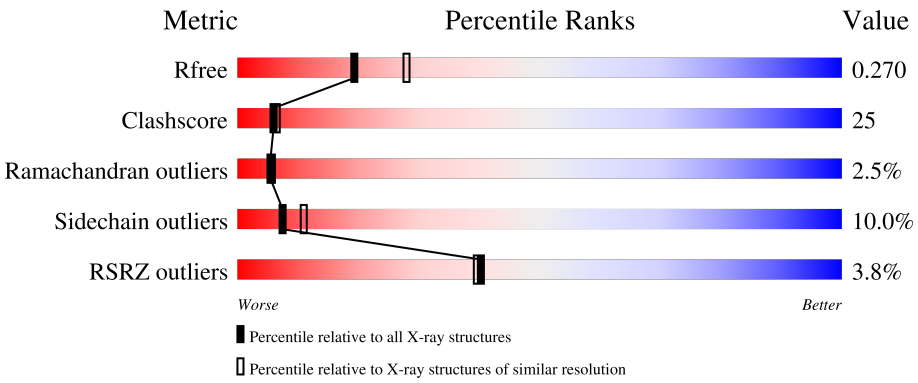
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	453	% 60% 30% 5% • •
1	B	453	7% 53% 36% 6% • •

2 Entry composition (i)

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

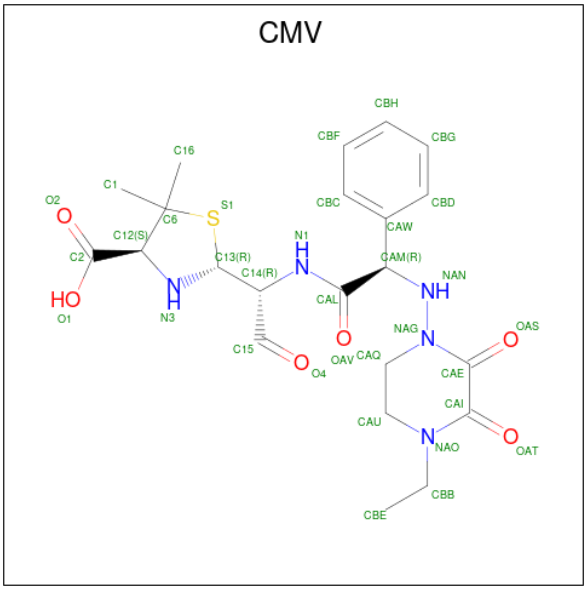
- Molecule 1 is a protein called Penicillin-binding protein 4.

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

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-carboxylic acid (three-letter code: CMV) (formula: $C_{22}H_{29}N_5O_6S$).



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

- Molecule 3 is water.

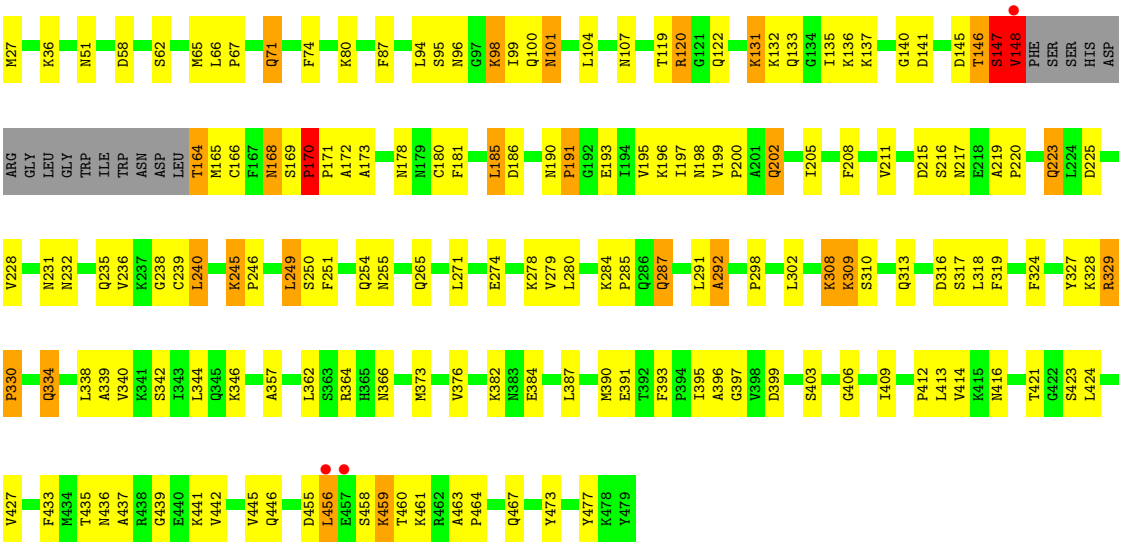
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	60	60	60	0	0
			Total	O		
3	B	26	26	26	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

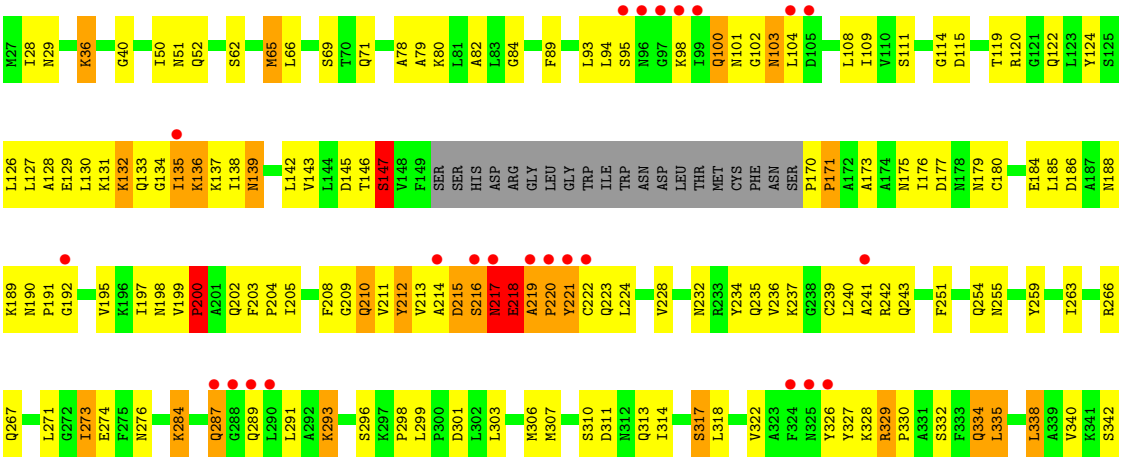
• Molecule 1: Penicillin-binding protein 4

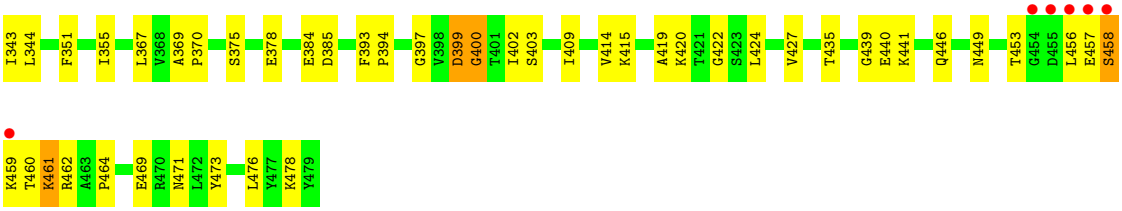
Chain A:



• Molecule 1: Penicillin-binding protein 4

Chain B:




I343
L344
F351
I355
L367
V368
A369
P370
S375
E378
E384
D385
F393
P394
G397
V398
D399
G400
T401
I402
S403
I409
V414
K415
A419
K420
T421
G422
S423
L424
V427
T435
G439
E440
K441
Q446
N449
T453
G454
D455
L456
E457
S458
K459
T460
K461
R462
A463
P464
E469
R470
N471
L472
Y473
L476
Y477
K478
Y479

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.20 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.217 , 0.280 0.215 , 0.270	Depositor DCC
R_{free} test set	2163 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6865	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 25.

All (341) 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)
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ASP:O	1:B:217:ASN:N	1.77	1.16
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:H	1:A:456:LEU:HD23	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: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	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:165:MET:HG3	1:A:166:CYS:H	1.41	0.85
1:B:131:LYS:O	1:B:134:GLY:N	2.07	0.85
1:B:191:PRO:HA	1:B:213:VAL:HG12	1.58	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:OE1	1:A:223:GLN:HA	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:HA	1:B:287:GLN:NE2	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:HD12	1:B:185:LEU:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:VAL:HG21	1:B:254:GLN:HG3	1.72	0.72
1:B:241:ALA:O	1:B:243:GLN:HG3	1.90	0.72
1:B:334:GLN:CD	1:B:334:GLN:H	1.91	0.72
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:CA	1:A:287:GLN:OE1	2.39	0.69
1:B:457:GLU:O	1:B:458:SER:HB3	1.92	0.69
1:A:202:GLN:HE21	1:A:202:GLN:N	1.87	0.69
1:B:223:GLN:HG2	1:B:224:LEU:N	2.07	0.69
1:A:74:PHE:CE1	1:A:376:VAL:HG21	2.27	0.69
1:B:28:ILE:HD11	1:B:476:LEU:HD23	1.75	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:A:137:LYS:HB2	1:A:274:GLU:HB3	1.75	0.67
1:B:216:SER:C	1:B:218:GLU:H	1.98	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:C	1:A:205:ILE:HD12	2.16	0.66
1:A:107:ASN:OD1	1:A:141:ASP:N	2.28	0.66
1:B:274:GLU:HG3	1:B:276:ASN:HD21	1.59	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:191:PRO:HB3	1:B:215:ASP:CA	2.23	0.63
1:B:223:GLN:CG	1:B:224:LEU:H	2.06	0.63
1:B:146:THR:HG22	1:B:147:SER:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:412:PRO:HG3	1:A:477:TYR:CD2	2.36	0.60
1:B:318:LEU:O	1:B:322:VAL:HG23	2.01	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:N	1:B:185:LEU:CD1	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:A:327:TYR:O	1:A:329:ARG:HG2	2.03	0.59
1:B:394:PRO:HB2	1:B:402:ILE:HG12	1.85	0.59
1:B:188:ASN:OD1	1:B:242:ARG:NH2	2.35	0.58
1:B:212:TYR:CD2	1:B:212:TYR:C	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
2:A:1:CMV:HAQ	2:A:1:CMV:OAV	2.04	0.56
1:B:52:GLN:NE2	1:B:440:GLU:OE2	2.37	0.56
1:B:89:PHE:N	1:B:296:SER:OG	2.35	0.56
1:B:180:CYS:HB2	1:B:251:PHE:O	2.05	0.56
2:A:1:CMV:CBE	2:A:1:CMV:OAT	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:131:LYS:HG3	1:B:273:ILE:HD11	1.89	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
1:A:421:THR:OG1	2:A:1:CMV:O1	2.23	0.53
1:A:215:ASP:O	1:A:219:ALA:HB2	2.08	0.53
1:A:456:LEU:H	1:A:456:LEU:CD2	2.08	0.53
1:A:216:SER:HA	1:A:219:ALA:CB	2.39	0.53
1:A:287:GLN:OE1	1:A:287:GLN:N	2.41	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:A:190:ASN:O	1:A:193:GLU:HG3	2.10	0.51
1:B:214:ALA:O	1:B:216:SER:N	2.35	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: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:436:ASN:HA	1:A:477:TYR:HD1	1.76	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:CD	1:B:334:GLN:N	2.60	0.50
1:A:27:MET:HE1	1:A:58:ASP:HB3	1.94	0.50
1:A:364:ARG:HD3	3:B:487:HOH:O	2.11	0.50
1:B:307:MET:CE	1:B:420:LYS:HD3	2.41	0.50
1:A:435:THR:HG22	1:A:439:GLY:HA2	1.93	0.50
1:B:188:ASN:O	1:B:189:LYS:HD2	2.11	0.50
1:B:114:GLY:O	1:B:115:ASP:C	2.50	0.49
1:B:109:ILE:HA	1:B:143:VAL:O	2.13	0.49
1:B:131:LYS:C	1:B:133:GLN:N	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:74:PHE:CD1	1:A:376:VAL:HG21	2.49	0.48
1:B:274:GLU:HG3	1:B:276:ASN:ND2	2.25	0.48
1:B:216:SER:C	1:B:218:GLU:N	2.65	0.48
1:A:291:LEU:O	1:A:292:ALA:HB2	2.14	0.47
1:A:399:ASP:OD1	1:A:399:ASP:C	2.52	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:84:GLY:O	1:B:299:LEU:HD22	2.14	0.47
1:B:228:VAL:HG21	1:B:254:GLN:CG	2.43	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:79:ALA:HB1	1:B:299:LEU:HD11	1.96	0.46
1:B:209:GLY:O	1:B:210:GLN:HG2	2.12	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:A:265:GLN:NE2	1:A:279:VAL:CG2	2.80	0.45
1:B:146:THR:CG2	1:B:147:SER:H	2.30	0.45
1:B:214:ALA:C	1:B:216:SER:H	2.16	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:A:216:SER:HA	1:A:219:ALA:HB3	1.99	0.45
1:B:327:TYR:OH	1:B:338:LEU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:66:LEU:HA	1:A:67:PRO:HD2	1.83	0.44
1:A:87:PHE:O	1:A:298:PRO:HA	2.17	0.44
1:B:145:ASP:OD1	1:B:145:ASP:C	2.56	0.44
1:B:186:ASP:O	1:B:195:VAL:HG13	2.17	0.44
1:B:311:ASP:OD1	1:B:314:ILE:HG13	2.17	0.44
1:B:414:VAL:O	1:B:414:VAL:CG1	2.65	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:A:231:ASN:CG	1:A:231:ASN:O	2.56	0.44
1:B:203:PHE:HB3	1:B:205:ILE:HG12	1.99	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:HB2	1:B:293:LYS:HE3	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:O	1:B:414:VAL:HG13	2.19	0.43
1:B:284:LYS:HE2	1:B:284:LYS:HB3	1.58	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:A:107:ASN:OD1	1:A:140:GLY:HA3	2.19	0.43
1:A:436:ASN:C	1:A:436:ASN:OD1	2.56	0.43
1:B:69:SER:HB2	1:B:422:GLY:HA2	2.00	0.43
1:A:463:ALA:N	1:A:464:PRO:CD	2.82	0.43
1:B:66:LEU:N	1:B:449:ASN:HD21	2.06	0.43
1:A:62:SER:O	1:B:40:GLY:HA2	2.19	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:446:GLN:O	1:A:446:GLN:HG2	2.19	0.42
1:B:93:LEU:HD11	1:B:126:LEU:O	2.18	0.42
1:A:249:LEU:HD23	1:A:249:LEU:HA	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:O	1:B:130:LEU:HB2	2.19	0.42
1:A:232:ASN:ND2	1:A:255:ASN:H	2.05	0.42
1:A:319:PHE:CE1	1:A:340:VAL:HG21	2.54	0.42
1:B:84:GLY:O	1:B:299:LEU:CD2	2.67	0.42
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.92	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
1:B:108:LEU:O	1:B:142:LEU:HD12	2.20	0.42
1:A:346:LYS:HB3	1:A:346:LYS:HE2	1.60	0.42
1:A:433:PHE:HA	1:A:442:VAL:O	2.20	0.42
1:B:28:ILE:HG22	1:B:29:ASN:N	2.34	0.42
1:B:222:CYS:SG	1:B:239:CYS:C	2.98	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:N	1:B:234:TYR:CD2	2.88	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:393:PHE:HA	1:B:394:PRO:HD2	1.87	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:A:437:ALA:HA	1:A:477:TYR:CE1	2.55	0.41
1:B:211:VAL:HG23	1:B:236:VAL:HG23	2.02	0.41
1:A:423:SER:O	1:A:424:LEU:HD23	2.20	0.41
1:A:459:LYS:H	1:A:459:LYS:HG3	1.52	0.41
1:B:78:ALA:HB2	1:B:340:VAL:HG13	2.03	0.41
1:B:119:THR:OG1	1:B:122:GLN:HG3	2.21	0.41
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.86	0.41
1:B:399:ASP:O	1:B:400:GLY:O	2.39	0.41
1:A:178:ASN:HA	1:A:313:GLN:HE22	1.85	0.41
1:A:285:PRO:HB3	3:A:7:HOH:O	2.20	0.41
1:B:28:ILE:CG2	1:B:29:ASN:N	2.82	0.41
1:B:222:CYS:SG	1:B:239:CYS:O	2.78	0.41
1:B:335:LEU:HD13	1:B:335:LEU:HA	1.90	0.41
1:B:369:ALA:O	1:B:370:PRO:C	2.59	0.41
1:A:119:THR:OG1	1:A:122:GLN:HG3	2.20	0.41
1:A:334:GLN:CD	1:A:334:GLN:H	2.20	0.40
1:B:101:ASN:C	1:B:103:ASN:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:VAL:HA	1:A:238:GLY:O	2.21	0.40
1:B:338:LEU:HD12	1:B:338:LEU:HA	1.89	0.40
1:A:185:LEU:CD2	1:A:197:ILE:HG23	2.49	0.40
1:B:184:GLU:OE1	1:B:198:ASN:HB2	2.22	0.40
1:A:327:TYR:CE2	1:A:339:ALA:HB2	2.57	0.40
2:A:1:CMV:OAT	2:A:1:CMV:HBEA	2.21	0.40
1:B:128:ALA:C	1:B:130:LEU:N	2.74	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 (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	A	434/453 (96%)	406 (94%)	20 (5%)	8 (2%)	8 10
1	B	429/453 (95%)	384 (90%)	31 (7%)	14 (3%)	4 3
All	All	863/906 (95%)	790 (92%)	51 (6%)	22 (2%)	5 6

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

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Mol	Chain	Res	Type
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 (i)

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%)	8 11
1	B	358/378 (95%)	322 (90%)	36 (10%)	7 11
All	All	723/756 (96%)	651 (90%)	72 (10%)	7 11

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	B	478	LYS

Sometimes 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

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Mol	Chain	Res	Type
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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	28,36,36	2.93	5 (17%)	38,52,52	2.81	13 (34%)
2	CMV	B	1	1	28,36,36	3.27	6 (21%)	38,52,52	2.09	15 (39%)

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	-	6/20/60/60	0/3/3/3
2	CMV	B	1	1	-	3/20/60/60	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	CMV	CAI-CAE	-13.59	1.31	1.53
2	A	1	CMV	CAI-CAE	-10.73	1.36	1.53
2	B	1	CMV	C6-S1	-7.44	1.70	1.85
2	A	1	CMV	C6-S1	-6.94	1.71	1.85
2	A	1	CMV	C13-S1	-5.73	1.71	1.84
2	A	1	CMV	CAW-CAM	-5.26	1.44	1.52
2	B	1	CMV	C13-S1	-4.92	1.73	1.84
2	A	1	CMV	CAM-CAL	-2.51	1.48	1.54
2	B	1	CMV	C14-N1	2.51	1.49	1.46
2	B	1	CMV	CAW-CAM	-2.24	1.49	1.52
2	B	1	CMV	O2-C2	2.08	1.28	1.22

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	CMV	CAE-NAG-NAN	-8.00	104.20	118.06
2	A	1	CMV	OAS-CAE-CAI	6.08	128.99	118.89
2	A	1	CMV	C1-C6-S1	5.59	118.19	109.18
2	A	1	CMV	CBB-NAO-CAI	5.09	125.68	119.59
2	A	1	CMV	CAL-CAM-NAN	4.93	123.69	108.58
2	A	1	CMV	CBC-CAW-CBD	4.58	123.98	118.30
2	B	1	CMV	C14-N1-CAL	-4.42	118.02	123.08
2	B	1	CMV	OAT-CAI-NAO	4.09	128.19	123.55
2	A	1	CMV	C16-C6-C1	-4.09	104.04	110.70
2	B	1	CMV	CBB-NAO-CAI	3.58	123.88	119.59
2	B	1	CMV	CAL-CAM-NAN	-3.44	98.04	108.58
2	A	1	CMV	C6-S1-C13	3.38	101.99	93.41
2	B	1	CMV	CAM-CAL-N1	3.33	125.36	116.84
2	A	1	CMV	CAU-NAO-CBB	-3.15	111.02	116.63
2	B	1	CMV	OAV-CAL-CAM	-3.12	115.37	120.58
2	A	1	CMV	CBC-CAW-CAM	-3.07	115.87	120.78
2	B	1	CMV	C6-S1-C13	3.05	101.16	93.41
2	A	1	CMV	CBG-CBD-CAW	-3.05	117.00	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	CMV	C16-C6-S1	2.93	113.91	109.18
2	B	1	CMV	C2-C12-N3	-2.91	106.13	110.62
2	B	1	CMV	CAW-CAM-CAL	2.87	115.17	108.42
2	B	1	CMV	C16-C6-C1	-2.66	106.36	110.70
2	B	1	CMV	C6-C12-C2	2.60	117.29	112.37
2	B	1	CMV	CAE-NAG-NAN	-2.56	113.62	118.06
2	A	1	CMV	CAW-CAM-CAL	2.29	113.82	108.42
2	B	1	CMV	OAS-CAE-CAI	-2.23	115.19	118.89
2	A	1	CMV	CAU-CAQ-NAG	-2.18	104.62	112.01
2	B	1	CMV	OAV-CAL-N1	-2.11	119.17	122.96

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	CMV	CAL-CAM-NAN-NAG
2	A	1	CMV	CBE-CBB-NAO-CAU
2	A	1	CMV	CBE-CBB-NAO-CAI
2	B	1	CMV	CAL-CAM-NAN-NAG
2	B	1	CMV	CBE-CBB-NAO-CAU
2	B	1	CMV	CBE-CBB-NAO-CAI
2	A	1	CMV	C15-C14-N1-CAL
2	A	1	CMV	N3-C12-C2-O2
2	A	1	CMV	N3-C12-C2-O1

There are no ring outliers.

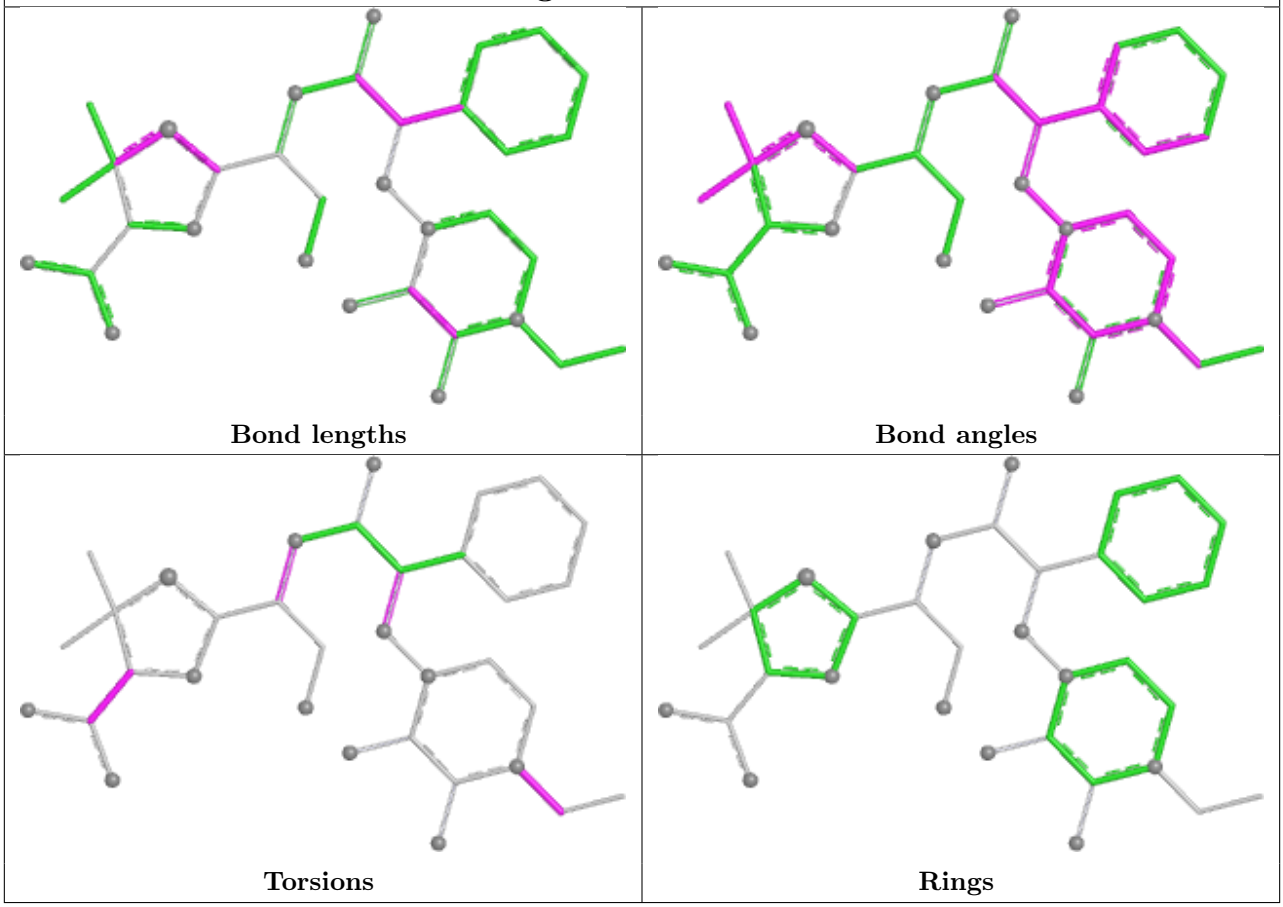
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	CMV	5	0

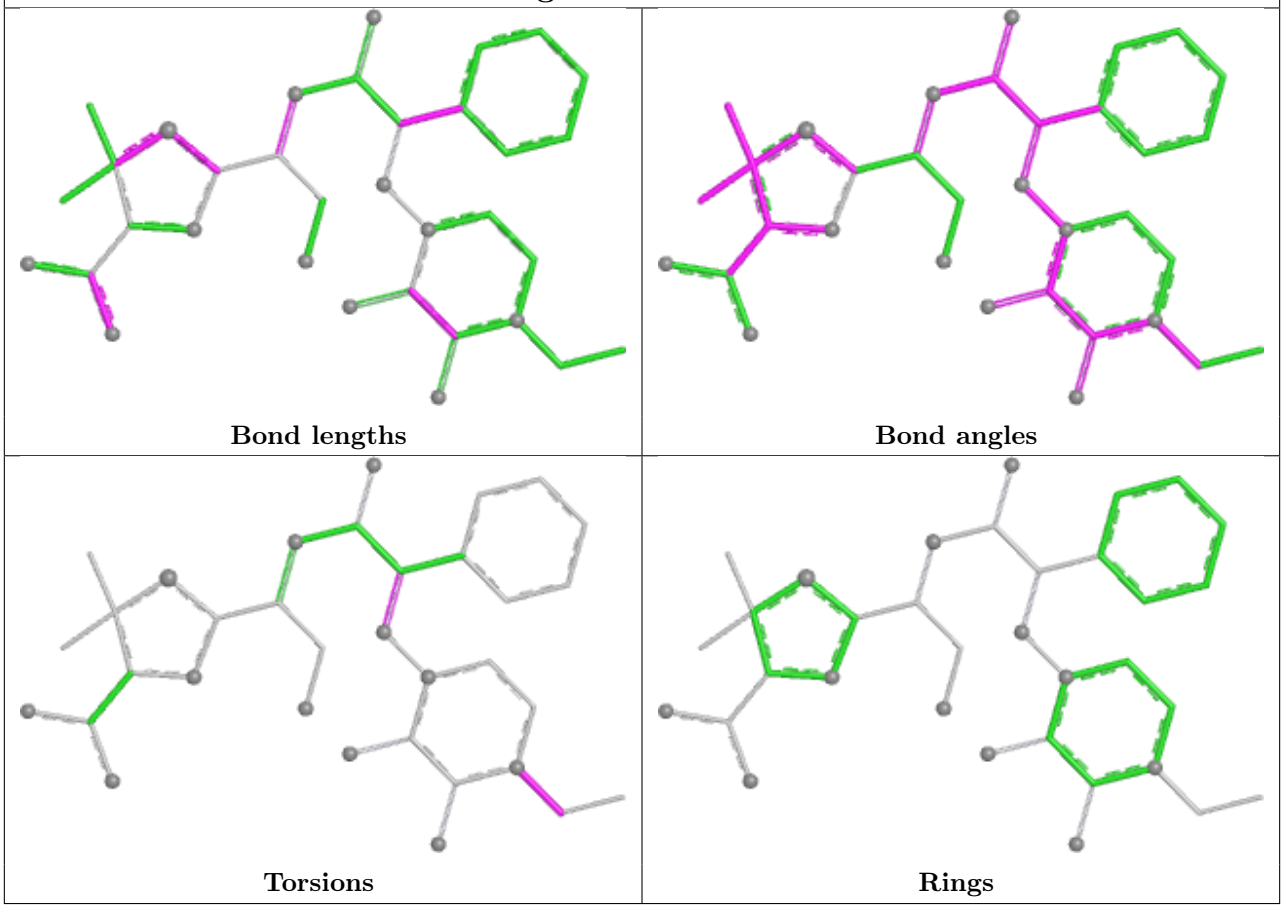
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand CMV A 1



Ligand CMV B 1



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	438/453 (96%)	0.05	3 (0%)	87	86	16, 32, 54, 76	0
1	B	433/453 (95%)	0.33	30 (6%)	16	15	18, 40, 72, 86	0
All	All	871/906 (96%)	0.18	33 (3%)	40	39	16, 36, 67, 86	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	456	LEU	7.5
1	B	217	ASN	4.7
1	B	287	GLN	4.7
1	B	220	PRO	4.7
1	B	96	ASN	4.4
1	B	98	LYS	4.1
1	B	457	GLU	4.0
1	A	456	LEU	3.9
1	B	222	CYS	3.9
1	B	221	TYR	3.7
1	B	288	GLY	3.6
1	B	326	TYR	3.2
1	A	148	VAL	3.2
1	B	289	GLN	3.1
1	B	216	SER	3.1
1	B	214	ALA	3.1
1	B	135	ILE	3.0
1	B	454	GLY	3.0
1	B	219	ALA	3.0
1	B	192	GLY	2.7
1	B	458	SER	2.7
1	A	457	GLU	2.7
1	B	455	ASP	2.6
1	B	459	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	95	SER	2.6
1	B	241	ALA	2.5
1	B	290	LEU	2.4
1	B	105	ASP	2.3
1	B	99	ILE	2.2
1	B	104	LEU	2.1
1	B	325	ASN	2.1
1	B	324	PHE	2.1
1	B	97	GLY	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

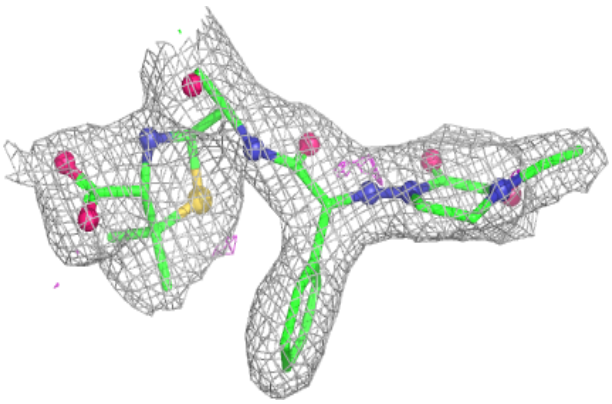
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

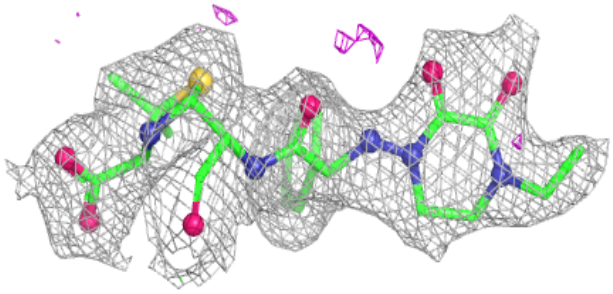
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CMV	B	1	34/34	0.94	0.14	25,33,54,57	0
2	CMV	A	1	34/34	0.96	0.15	15,25,46,47	0

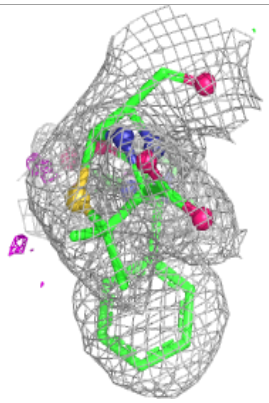
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CMV B 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

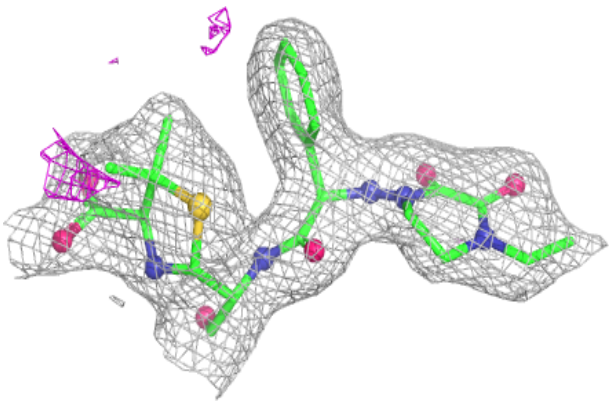


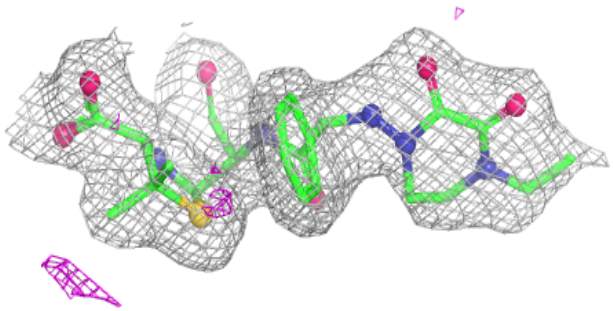


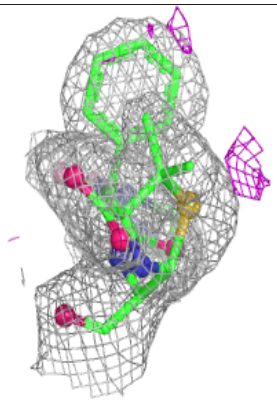


Electron density around CMV A 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.