



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:44 PM UTC

PDB ID : 3A3E / pdb_00003a3e
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

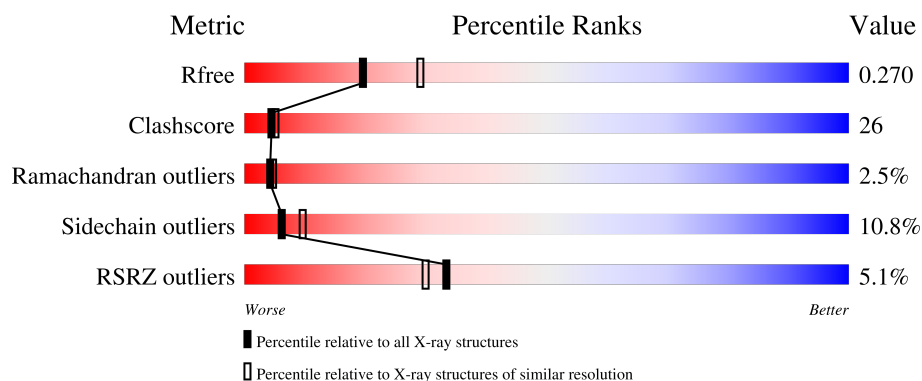
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	A	453	3% 55% 34% 7% ..
1	B	453	7% 45% 40% 9% ..

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.

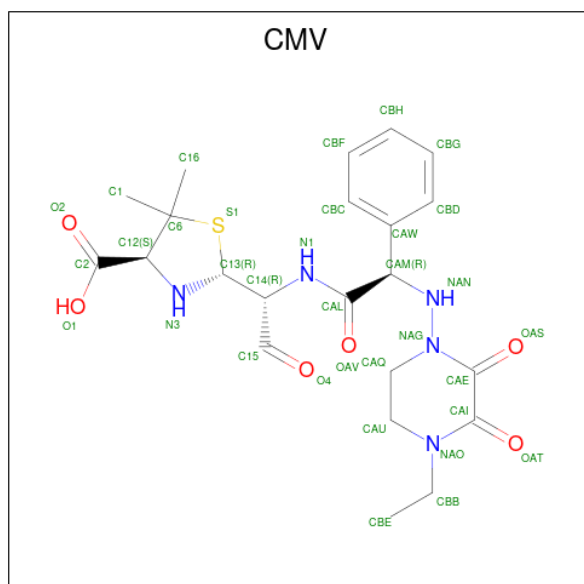
- Molecule 1 is a protein called Penicillin-binding protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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-carboxylic acid (CCD ID: CMV) (formula: C₂₂H₂₉N₅O₆S).



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		

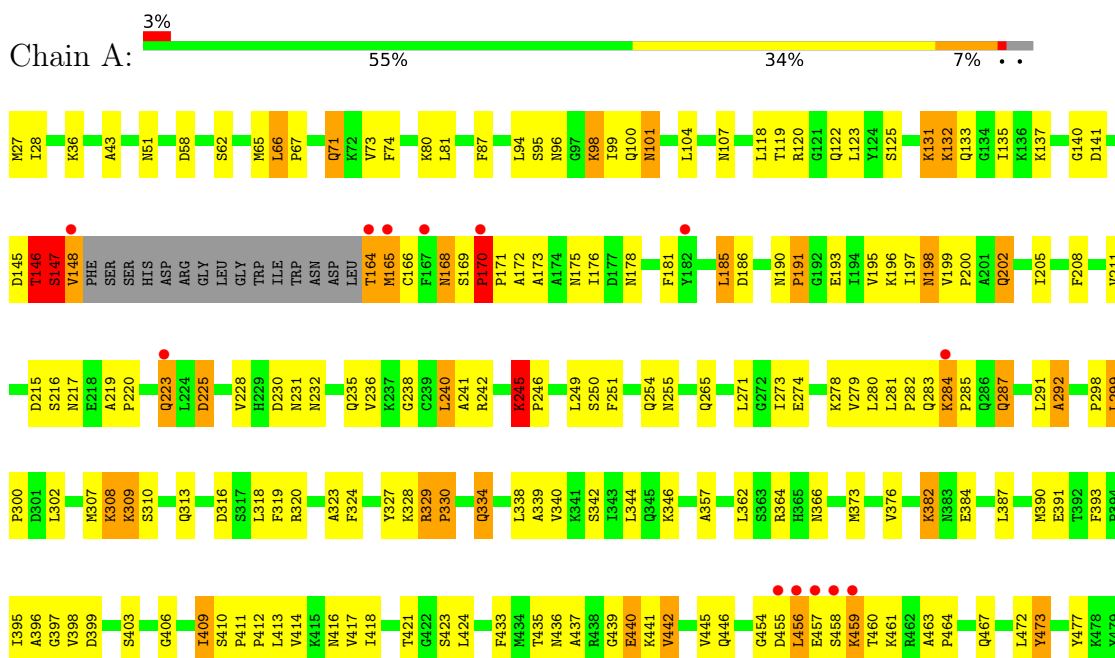
- Molecule 3 is water.

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

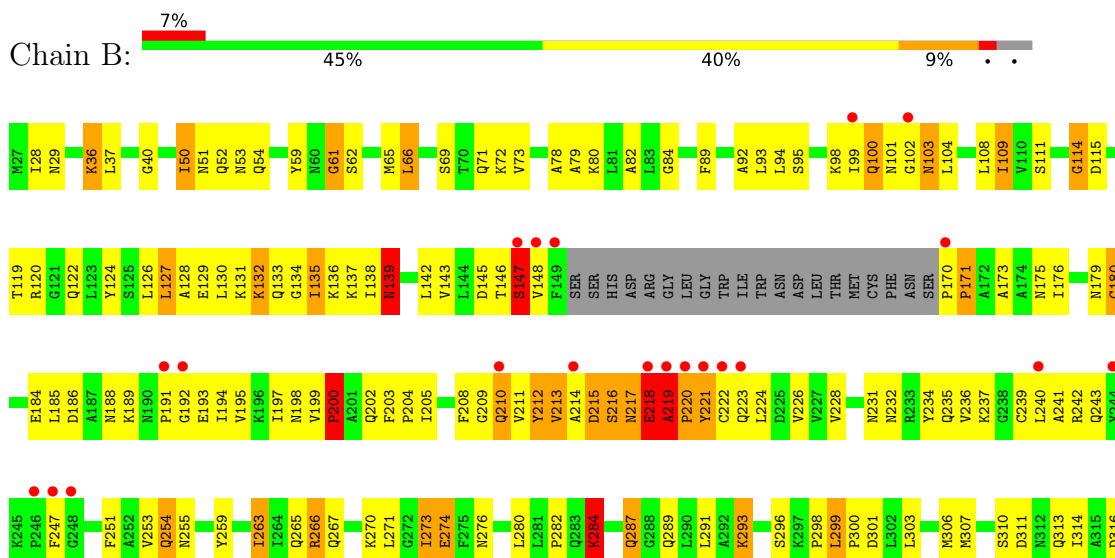
3 Residue-property plots

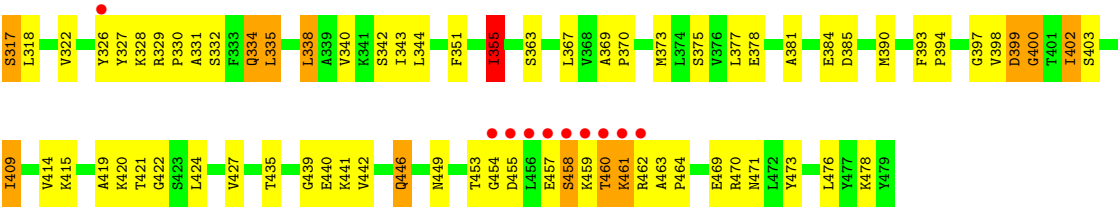
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Penicillin-binding protein 4





4 Data and refinement statistics

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 49.57 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.57-2.40) 93.0 (49.57-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.34 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	1.34	9/3437 (0.3%)	1.46	30/4644 (0.6%)
1	B	1.18	7/3391 (0.2%)	1.37	40/4582 (0.9%)
All	All	1.26	16/6828 (0.2%)	1.42	70/9226 (0.8%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	SER	CA-C	7.76	1.63	1.52
1	A	28	ILE	CA-CB	-7.68	1.46	1.54
1	B	460	THR	CA-CB	6.69	1.62	1.53
1	B	263	ILE	CA-CB	-6.13	1.47	1.54
1	B	253	VAL	CA-CB	5.79	1.61	1.54
1	A	418	ILE	CA-CB	-5.68	1.47	1.54
1	A	125	SER	CA-C	-5.60	1.45	1.52
1	A	442	VAL	CA-CB	-5.57	1.47	1.54
1	A	472	LEU	C-O	-5.41	1.17	1.24
1	A	176	ILE	CA-CB	-5.35	1.47	1.54
1	B	54	GLN	CA-C	5.17	1.58	1.52
1	B	355	ILE	CA-CB	-5.13	1.47	1.53
1	B	316	ASP	CA-C	-5.09	1.45	1.52
1	A	410	SER	C-O	5.06	1.28	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	GLY	C-O	5.04	1.30	1.23
1	A	43	ALA	CA-C	-5.00	1.46	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PRO	CA-C-N	-14.63	101.55	119.84
1	A	170	PRO	C-N-CA	-14.63	101.55	119.84
1	A	66	LEU	CA-C-N	9.54	129.20	119.56
1	A	66	LEU	C-N-CA	9.54	129.20	119.56
1	A	281	LEU	CA-C-N	8.94	128.68	119.56
1	A	281	LEU	C-N-CA	8.94	128.68	119.56
1	B	299	LEU	CA-C-N	-8.85	109.81	119.19
1	B	299	LEU	C-N-CA	-8.85	109.81	119.19
1	B	378	GLU	N-CA-C	-8.61	101.39	112.23
1	A	165	MET	N-CA-C	8.38	121.33	110.53
1	B	463	ALA	CA-C-N	-8.37	110.32	119.19
1	B	463	ALA	C-N-CA	-8.37	110.32	119.19
1	B	284	LYS	CA-C-N	-7.54	112.01	119.78
1	B	284	LYS	C-N-CA	-7.54	112.01	119.78
1	A	225	ASP	N-CA-C	7.42	120.20	109.14
1	B	247	PHE	N-CA-C	7.36	118.89	108.74
1	A	411	PRO	N-CA-C	-7.10	102.04	110.70
1	A	198	ASN	CA-C-N	-7.00	117.55	122.59
1	A	198	ASN	C-N-CA	-7.00	117.55	122.59
1	A	417	VAL	CB-CA-C	-6.98	101.97	111.33
1	B	66	LEU	CA-C-N	6.91	126.62	119.64
1	B	66	LEU	C-N-CA	6.91	126.62	119.64
1	B	266	ARG	N-CA-C	-6.86	103.81	111.28
1	B	92	ALA	N-CA-C	6.83	120.77	108.69
1	B	109	ILE	CB-CA-C	-6.78	102.24	111.33
1	B	455	ASP	N-CA-C	6.64	118.43	110.19
1	A	282	PRO	N-CA-C	6.62	122.45	113.84
1	A	230	ASP	N-CA-C	6.61	118.83	110.24
1	A	398	VAL	CB-CA-C	-6.56	104.48	110.91
1	B	409	ILE	N-CA-C	6.46	118.36	112.29
1	B	454	GLY	N-CA-C	6.42	122.85	110.66
1	A	284	LYS	CA-C-N	-6.06	113.54	119.78
1	A	284	LYS	C-N-CA	-6.06	113.54	119.78
1	B	398	VAL	CB-CA-C	-6.06	105.66	111.05
1	B	373	MET	N-CA-C	-6.05	104.61	111.14
1	B	219	ALA	CA-C-N	5.93	127.25	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	ALA	C-N-CA	5.93	127.25	119.84
1	B	254	GLN	CA-C-N	-5.88	113.77	122.41
1	B	254	GLN	C-N-CA	-5.88	113.77	122.41
1	B	363	SER	N-CA-C	5.85	118.81	110.10
1	B	139	ASN	N-CA-C	5.76	118.43	111.40
1	A	283	GLN	CA-C-N	-5.73	113.47	124.01
1	A	283	GLN	C-N-CA	-5.73	113.47	124.01
1	B	37	LEU	N-CA-C	-5.68	101.86	110.39
1	A	146	THR	N-CA-C	5.68	122.91	110.80
1	B	399	ASP	N-CA-C	5.68	115.60	108.45
1	A	123	LEU	N-CA-C	-5.60	105.25	111.36
1	B	226	VAL	CB-CA-C	-5.58	102.89	110.42
1	B	231	ASN	N-CA-C	5.52	119.24	111.52
1	A	473	TYR	CA-CB-CG	-5.51	103.97	113.90
1	B	194	ILE	N-CA-C	5.49	116.67	109.58
1	A	81	LEU	N-CA-C	5.43	117.28	111.36
1	B	180	CYS	N-CA-C	5.43	117.66	109.41
1	B	114	GLY	N-CA-C	-5.38	107.79	115.64
1	B	226	VAL	N-CA-C	5.34	115.68	107.77
1	A	299	LEU	CA-C-N	-5.28	113.31	119.32
1	A	299	LEU	C-N-CA	-5.28	113.31	119.32
1	B	470	ARG	N-CA-C	-5.24	105.26	110.97
1	A	454	GLY	N-CA-C	5.23	119.13	110.55
1	B	402	ILE	N-CA-C	5.23	117.43	111.88
1	A	175	ASN	CB-CA-C	-5.20	100.73	109.72
1	B	377	LEU	N-CA-C	5.18	116.93	111.28
1	B	442	VAL	CB-CA-C	-5.18	103.43	110.42
1	B	331	ALA	N-CA-C	5.12	117.06	107.99
1	B	148	VAL	N-CA-C	-5.09	101.31	109.20
1	A	118	LEU	N-CA-C	5.09	117.72	110.24
1	B	127	LEU	N-CA-C	-5.08	105.44	111.69
1	A	320	ARG	N-CA-C	5.07	116.88	111.36
1	B	421	THR	CB-CA-C	-5.05	101.71	110.45
1	A	245	LYS	N-CA-C	-5.04	98.67	109.81

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 ⓘ

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	157	0
1	B	3333	0	3400	205	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	361	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 26.

All (361) 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:218:GLU:C	1:B:220:PRO:HD2	1.53	1.33
1:B:218:GLU:C	1:B:220:PRO:CD	2.05	1.30
1:B:212:TYR:CE2	1:B:239:CYS:HB3	1.66	1.29
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
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:B:209:GLY:C	1:B:210:GLN:HG2	1.83	0.97
1:A:80:LYS:HE3	1:A:387:LEU:O	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:446:GLN:O	1:B:446:GLN:HG2	1.68	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
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:A:329:ARG:O	1:A:330:PRO:C	2.23	0.82
1:B:215:ASP:C	1:B:217:ASN:H	1.87	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:184:GLU:C	1:B:185:LEU:HD12	2.07	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: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:334:GLN:CD	1:B:334:GLN:H	1.91	0.76
1:B:298:PRO:HD2	1:B:301:ASP:OD2	1.86	0.75
1:B:208:PHE:CZ	1:B:235:GLN:HB2	2.23	0.74
1:B:218:GLU:C	1:B:220:PRO:HD3	1.94	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
1:B:216:SER:C	1:B:218:GLU:H	1.98	0.72
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: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:A:205:ILE:C	1:A:205:ILE:HD12	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:94:LEU:C	1:B:291:LEU:HD12	2.18	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: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: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:B:124:TYR:HH	1:B:271:LEU:HD23	1.59	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:199:VAL:O	1:B:200:PRO:C	2.39	0.64
1:B:212:TYR:C	1:B:212:TYR:HD2	2.05	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
1:B:212:TYR:CD2	1:B:212:TYR:C	2.77	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
1:B:215:ASP:C	1:B:217:ASN:N	2.49	0.62
1:B:131:LYS:O	1:B:132:LYS:C	2.40	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLY:HA2	1:B:136:LYS:HG3	1.81	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:B:334:GLN:CD	1:B:334:GLN:N	2.60	0.59
1:A:185:LEU:HD21	1:A:197:ILE:HG23	1.83	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: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:381:ALA:HA	1:B:390:MET:HE2	1.86	0.57
1:A:131:LYS:CE	1:A:271:LEU:O	2.52	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:329:ARG:C	1:A:330:PRO:O	2.49	0.55
1:B:218:GLU:O	1:B:220:PRO:HD2	1.99	0.55
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:114:GLY:O	1:B:115:ASP:C	2.50	0.54
1:B:327:TYR:O	1:B:328:LYS:HB2	2.06	0.54
1:B:131:LYS:C	1:B:133:GLN:N	2.63	0.54
1:B:313:GLN:O	1:B:317:SER:OG	2.26	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:131:LYS:HG3	1:B:273:ILE:HD11	1.89	0.54
1:A:436:ASN:C	1:A:477:TYR:CE1	2.86	0.54
1:B:127:LEU:HD12	1:B:267:GLN:OE1	2.08	0.54
1:A:190:ASN:O	1:A:191:PRO:C	2.51	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:27:MET:HE1	1:A:58:ASP:CB	2.38	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:A:399:ASP:OD1	1:A:399:ASP:C	2.52	0.52
1:B:146:THR:CG2	1:B:147:SER:N	2.72	0.52
1:B:216:SER:C	1:B:218:GLU:N	2.65	0.52
1:B:102:GLY:HA2	1:B:134:GLY:O	2.09	0.52
1:A:145:ASP:OD1	1:A:145:ASP:C	2.52	0.52
1:A:382:LYS:HG3	1:A:382:LYS:O	2.08	0.52
1:A:27:MET:HE1	1:A:58:ASP:HB3	1.92	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:100:GLN:O	1:A:101:ASN:C	2.52	0.51
1:A:168:ASN:OD1	1:A:169:SER:N	2.45	0.50
1:B:214:ALA:C	1:B:216:SER:H	2.16	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:A:328:LYS:C	1:A:329:ARG:HG2	2.37	0.49
1:A:395:ILE:O	1:A:396:ALA:C	2.55	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:B:145:ASP:OD1	1:B:145:ASP:C	2.56	0.49
1:A:413:LEU:O	1:A:416:ASN:HB3	2.12	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:231:ASN:CG	1:A:231:ASN:O	2.56	0.49
1:A:362:LEU:HD22	2:A:1:CMV:HAU	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:PRO:O	1:B:205:ILE:HD13	2.12	0.49
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:72:LYS:HB3	1:B:306:MET:HE3	1.95	0.48
1:B:274:GLU:HG3	1:B:276:ASN:ND2	2.25	0.48
1:B:384:GLU:O	1:B:385:ASP:C	2.56	0.48
1:A:291:LEU:O	1:A:292:ALA:HB2	2.14	0.47
1:A:436:ASN:C	1:A:436:ASN:OD1	2.56	0.47
1:A:245:LYS:HB3	1:A:246:PRO:CD	2.44	0.47
1:B:222:CYS:SG	1:B:239:CYS:C	2.98	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:169:SER:O	1:A:170:PRO:C	2.56	0.47
1:B:307:MET:HE3	1:B:420:LYS:HD3	1.95	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: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: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: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
1:A:98:LYS:HE3	1:A:98:LYS:HB3	1.51	0.45
1:A:436:ASN:HA	1:A:477:TYR:CD1	2.51	0.45
1:A:334:GLN:CD	1:A:334:GLN:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ASN:O	1:B:53:ASN:CG	2.60	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:369:ALA:O	1:B:370:PRO:C	2.59	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:101:ASN:C	1:B:103:ASN:H	2.25	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:128:ALA:C	1:B:130:LEU:H	2.26	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:131:LYS:C	1:A:133:GLN:N	2.74	0.44
1:B:265:GLN:O	1:B:266:ARG:C	2.60	0.44
1:B:72:LYS:O	1:B:73:VAL:C	2.59	0.44
1:A:241:ALA:O	1:A:242:ARG:C	2.61	0.44
1:A:65:MET:O	1:A:67:PRO:HD3	2.18	0.43
1:A:205:ILE:C	1:A:205:ILE:CD1	2.86	0.43
1:B:128:ALA:C	1:B:130:LEU:N	2.74	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:280:LEU:C	1:B:282:PRO:HD3	2.44	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:A:107:ASN:OD1	1:A:140:GLY:HA3	2.19	0.43
1:A:131:LYS:O	1:A:132:LYS:C	2.61	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:B:93:LEU:HD11	1:B:126:LEU:O	2.18	0.42
1:B:306:MET:HB3	1:B:306:MET:HE2	1.76	0.42
1:A:73:VAL:HG22	1:A:307:MET:HE1	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:127:LEU:O	1:B:130:LEU:HB2	2.19	0.42
1:B:311:ASP:CG	1:B:314:ILE:HG13	2.44	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:B:399:ASP:C	1:B:399:ASP:OD1	2.61	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: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:A:299:LEU:O	1:A:300:PRO:C	2.63	0.41
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:28:ILE:HG22	1:B:29:ASN:N	2.34	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:323:ALA:O	1:A:324:PHE:C	2.63	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:59:TYR:C	1:B:61:GLY:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:119:THR:OG1	1:A:122:GLN:HG3	2.20	0.41
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:B:299:LEU:O	1:B:300:PRO:C	2.63	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:A:51:ASN:CG	1:A:440:GLU:HB3	2.47	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%)	6	9
1	B	429/453 (95%)	384 (90%)	31 (7%)	14 (3%)	3	2
All	All	863/906 (95%)	790 (92%)	51 (6%)	22 (2%)	4	5

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

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Mol	Chain	Res	Type
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%)	327 (90%)	38 (10%)	7	10
1	B	358/378 (95%)	318 (89%)	40 (11%)	6	9
All	All	723/756 (96%)	645 (89%)	78 (11%)	6	9

All (78) 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	147	SER
1	A	148	VAL
1	A	164	THR

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Mol	Chain	Res	Type
1	A	168	ASN
1	A	185	LEU
1	A	202	GLN
1	A	223	GLN
1	A	240	LEU
1	A	245	LYS
1	A	250	SER
1	A	273	ILE
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	318	LEU
1	A	329	ARG
1	A	334	GLN
1	A	338	LEU
1	A	342	SER
1	A	382	LYS
1	A	391	GLU
1	A	409	ILE
1	A	414	VAL
1	A	440	GLU
1	A	455	ASP
1	A	456	LEU
1	A	457	GLU
1	A	458	SER
1	A	459	LYS
1	A	460	THR
1	A	461	LYS
1	B	36	LYS
1	B	50	ILE
1	B	62	SER
1	B	71	GLN
1	B	98	LYS
1	B	99	ILE
1	B	100	GLN
1	B	103	ASN
1	B	111	SER
1	B	135	ILE
1	B	139	ASN

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Mol	Chain	Res	Type
1	B	193	GLU
1	B	200	PRO
1	B	210	GLN
1	B	212	TYR
1	B	213	VAL
1	B	218	GLU
1	B	237	LYS
1	B	270	LYS
1	B	273	ILE
1	B	274	GLU
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	334	GLN
1	B	335	LEU
1	B	338	LEU
1	B	342	SER
1	B	355	ILE
1	B	375	SER
1	B	409	ILE
1	B	446	GLN
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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	51	ASN
1	A	53	ASN
1	A	103	ASN
1	A	139	ASN
1	A	198	ASN
1	A	202	GLN
1	A	232	ASN
1	A	283	GLN

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Mol	Chain	Res	Type
1	A	334	GLN
1	A	366	ASN
1	A	383	ASN
1	A	446	GLN
1	B	51	ASN
1	B	71	GLN
1	B	103	ASN
1	B	139	ASN
1	B	179	ASN
1	B	217	ASN
1	B	232	ASN
1	B	235	GLN
1	B	276	ASN
1	B	286	GLN
1	B	287	GLN
1	B	294	HIS
1	B	383	ASN
1	B	449	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 oligosaccharides 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(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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:

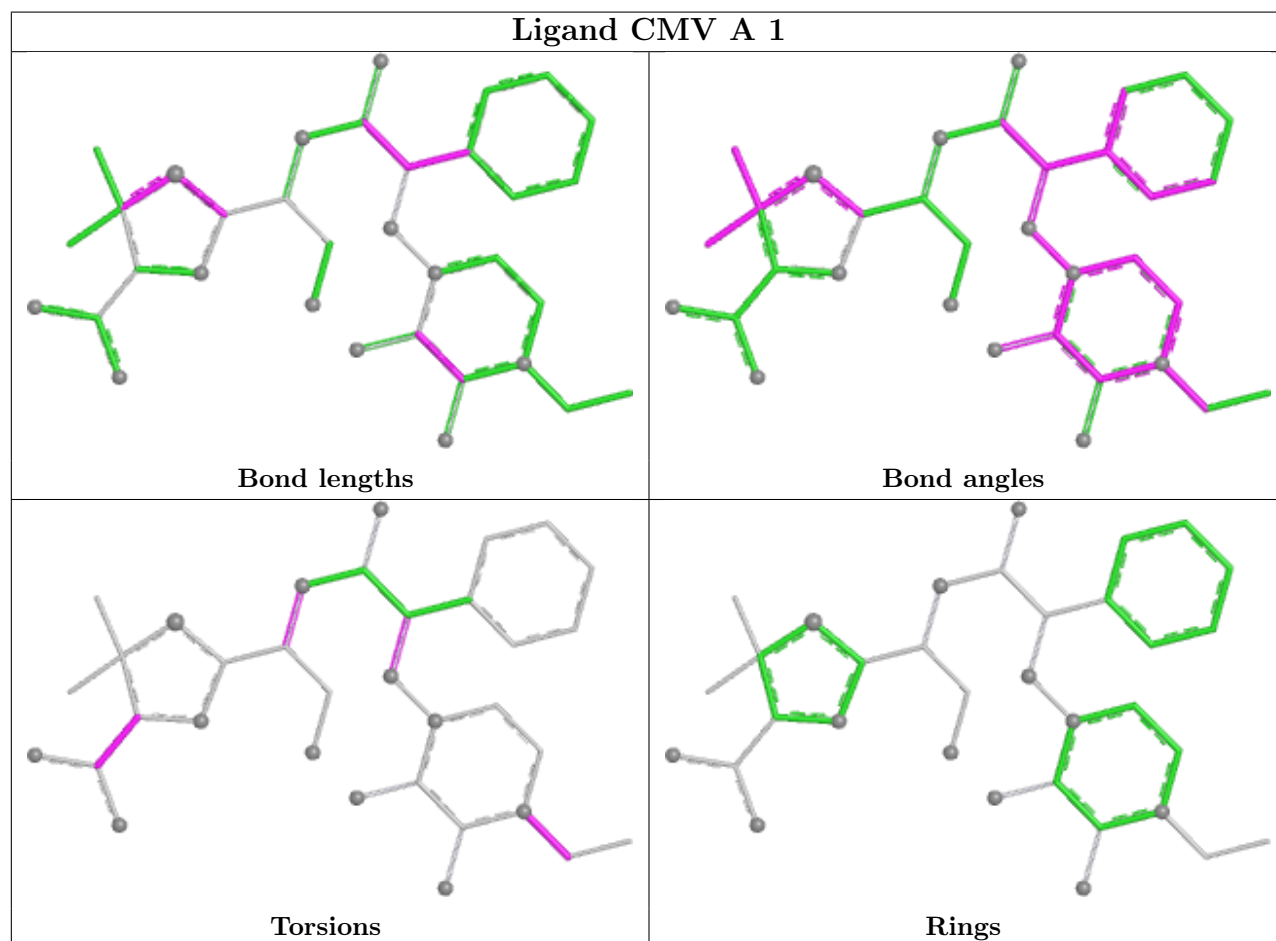
Mol	Chain	Res	Type	Atoms
2	A	1	CMV	CAL-CAM-NAN-NAG
2	A	1	CMV	CBE-CBB-NAO-CAU
2	A	1	CMV	CBE-CBB-NAO-CAI
2	B	1	CMV	CAL-CAM-NAN-NAG
2	B	1	CMV	CBE-CBB-NAO-CAU
2	B	1	CMV	CBE-CBB-NAO-CAI
2	A	1	CMV	C15-C14-N1-CAL
2	A	1	CMV	N3-C12-C2-O2
2	A	1	CMV	N3-C12-C2-O1

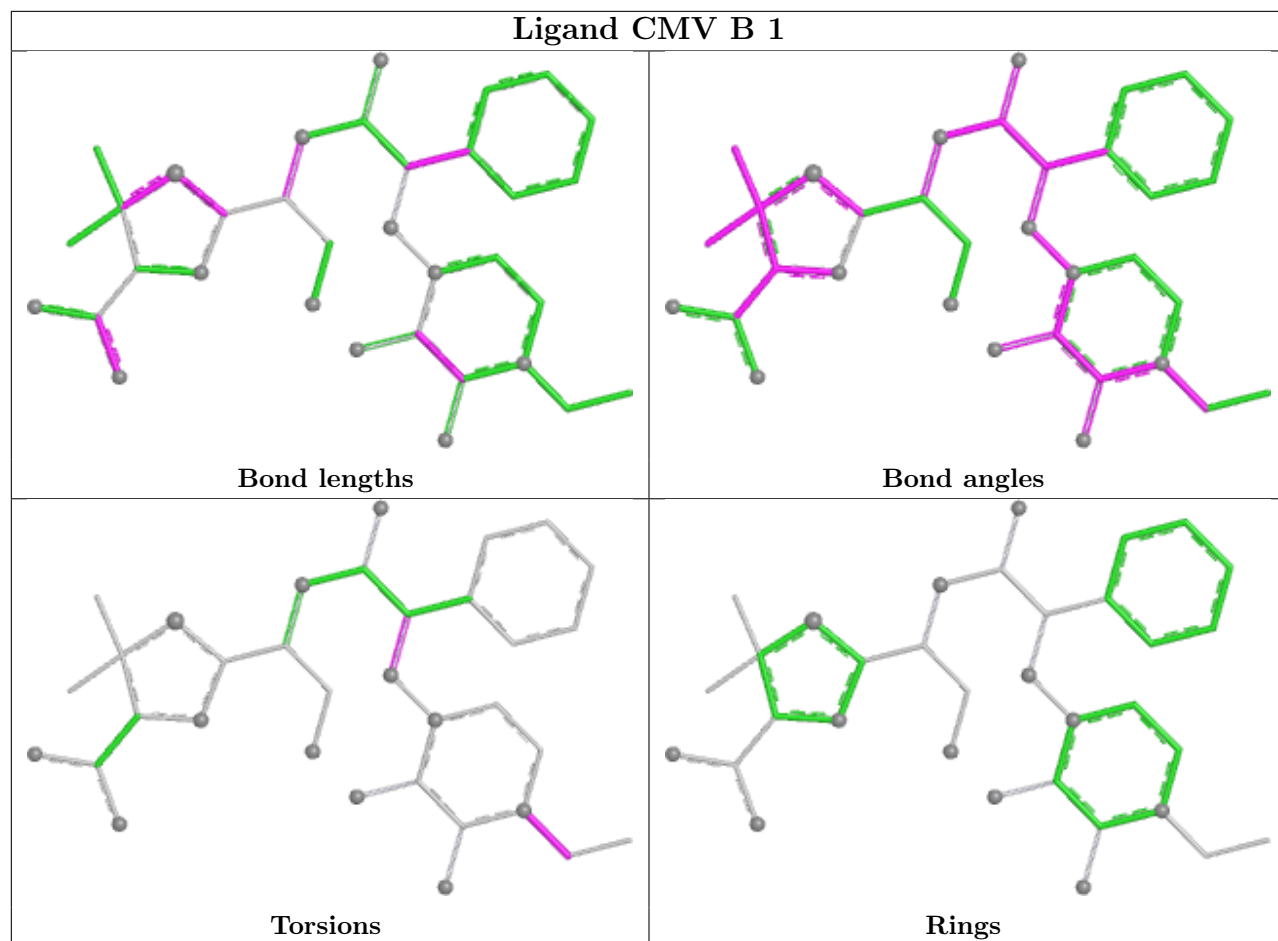
There are no ring outliers.

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 than 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.





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, 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%)	-0.15	13 (2%) 52 48	16, 32, 54, 76	0
1	B	433/453 (95%)	0.36	31 (7%) 21 18	18, 40, 72, 86	0
All	All	871/906 (96%)	0.10	44 (5%) 33 30	16, 36, 67, 86	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	456	LEU	9.2
1	A	456	LEU	5.7
1	B	457	GLU	5.2
1	B	459	LYS	4.8
1	B	149	PHE	4.5
1	B	460	THR	4.2
1	B	220	PRO	4.1
1	A	457	GLU	4.1
1	A	165	MET	4.1
1	B	222	CYS	4.1
1	B	219	ALA	4.0
1	B	454	GLY	3.9
1	A	164	THR	3.9
1	B	221	TYR	3.8
1	B	326	TYR	3.8
1	A	148	VAL	3.3
1	B	170	PRO	3.2
1	B	458	SER	3.2
1	B	223	GLN	3.1
1	A	455	ASP	3.1
1	B	148	VAL	3.1
1	B	461	LYS	2.8
1	A	167	PHE	2.8
1	B	99	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	214	ALA	2.8
1	B	455	ASP	2.7
1	B	247	PHE	2.6
1	A	170	PRO	2.6
1	A	459	LYS	2.5
1	B	147	SER	2.5
1	B	248	GLY	2.5
1	B	246	PRO	2.4
1	A	458	SER	2.3
1	B	244	TYR	2.3
1	B	192	GLY	2.3
1	B	462	ARG	2.3
1	B	218	GLU	2.2
1	B	102	GLY	2.2
1	A	223	GLN	2.1
1	A	284	LYS	2.1
1	B	240	LEU	2.1
1	B	210	GLN	2.1
1	A	182	TYR	2.1
1	B	191	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

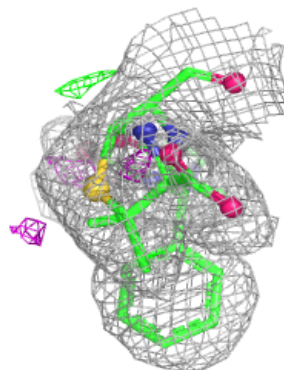
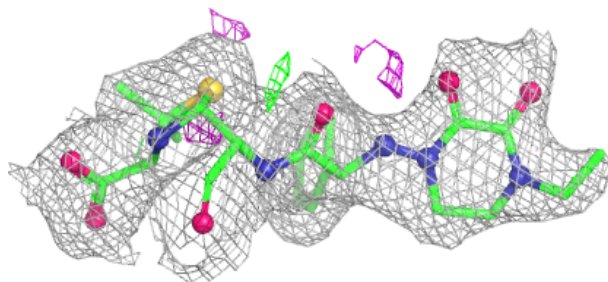
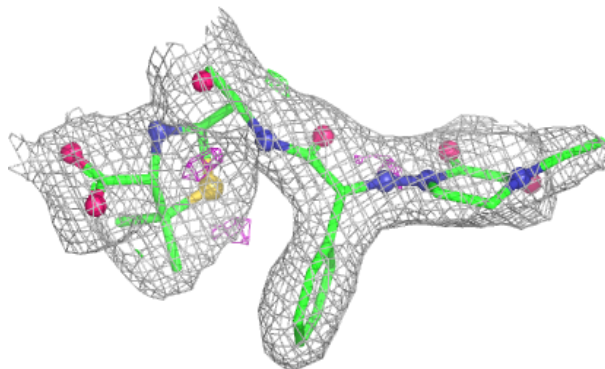
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.92	0.10	25,33,54,57	0
2	CMV	A	1	34/34	0.96	0.07	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.

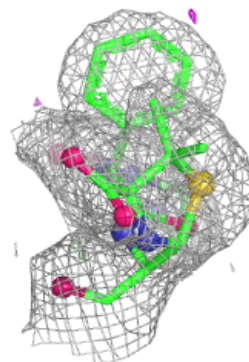
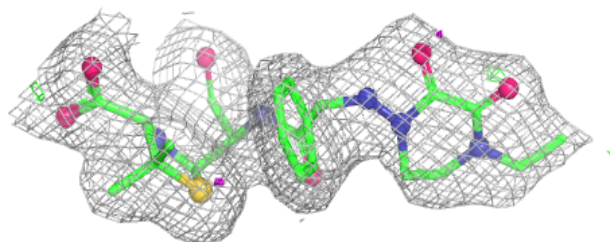
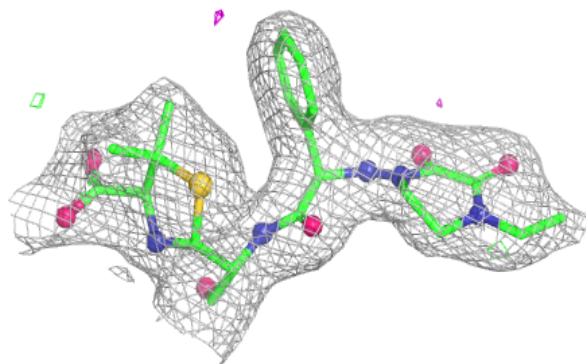
Electron density around CMV B 1:

$2mF_o-DF_c$ (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.