Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 07:30 PM EST

PDB ID	:	3B03
Title	:	Crystal structure of Sulfolobus shibatae isopentenyl diphosphate isomerase in complex with vIPP.
Authors	:	Unno, H.; Nagai, T.; Hemmi, H.
Deposited on	:	2011-06-03
Resolution	:	2.20 Å(reported)

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

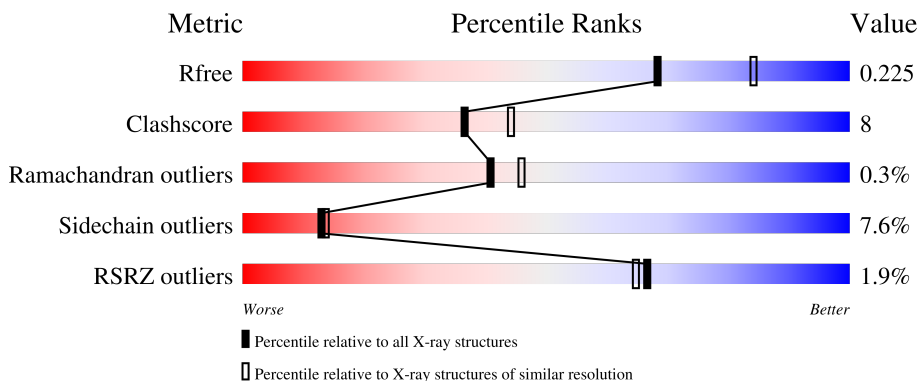|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	Percentile Ranks	Value
Rfree		0.225
Clashscore		8
Ramachandran outliers		0.3%
Sidechain outliers		7.6%
RSRZ outliers		1.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	368	2% 80% 15% • •
1	B	368	2% 82% 14% • •
1	C	368	2% 79% 17% • •
1	D	368	2% 83% 13% • •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 11968 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 Isopentenyl-diphosphate delta-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2803	1795	477	520	11			
1	B	364	Total	C	N	O	S	0	0	0
			2811	1801	478	521	11			
1	C	364	Total	C	N	O	S	0	0	0
			2811	1801	478	521	11			
1	D	364	Total	C	N	O	S	0	0	0
			2811	1801	478	521	11			

- Molecule 2 is 1-deoxy-1-[(4aR)-4a-[(2Z)-2-(2-{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy} ethyl)but-2-en-1-yl]-7,8-dimethyl-2,4-dioxo-3,4,4a,5-tetrahydrobenzo[g]pteridin-10(2H)-yl]-5 -O-phosphono-D-ribitol (three-letter code: VNR) (formula: $C_{23}H_{35}N_4O_{16}P_3$).
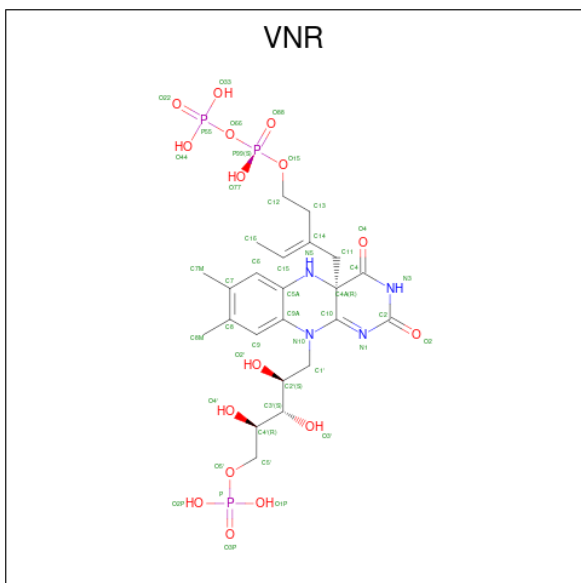
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			46	23	4	16	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			46	23	4	16	3		
2	C	1	Total	C	N	O	P	0	0
			46	23	4	16	3		
2	D	1	Total	C	N	O	P	0	0
			46	23	4	16	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	0
			124	124		
4	B	138	Total	O	0	0
			138	138		
4	C	146	Total	O	0	0
			146	146		
4	D	137	Total	O	0	0
			137	137		

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: Isopentenyl-diphosphate delta-isomerase
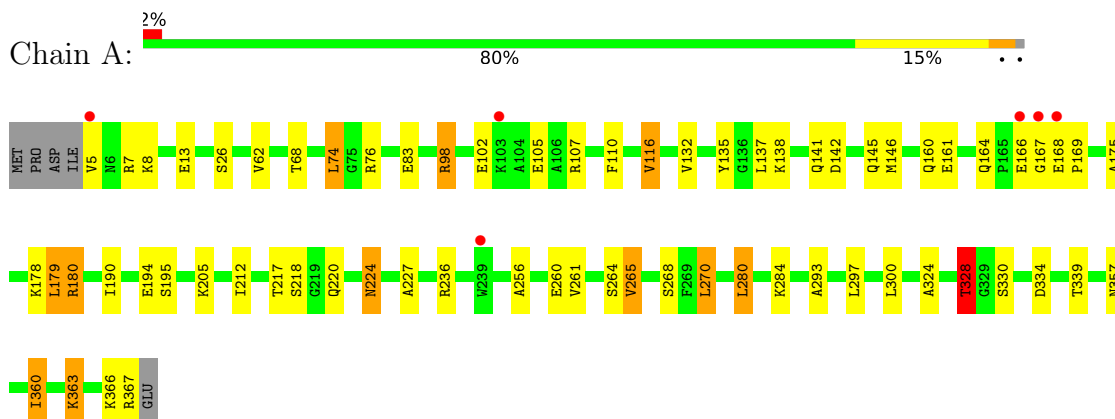
- Molecule 1: Isopentenyl-diphosphate delta-isomerase

- Molecule 1: Isopentenyl-diphosphate delta-isomerase

T328 D334 K338 Y353 N357 I360 Y361 E362 K363 V364 R365 K366 R367 GLU

• Molecule 1: Isopentenyl-diphosphate delta-isomerase

Chain D:

2%

83% 13%

MET PRO ASP I4 V5 N6 R7 K8 E13 I58 M67 T68 R71 N72 E73 L74 G75 R76 P91 R98 E102 K103 A104 E105 A106 R107 F110 V116 V132 L137 Q145 M146 Q160 E161 Q164 P165 E166 G167 E168 P169 A175 L179 R180

E185 I190 E194 S195 I212 R232 R235 R236 A256 E260 V261 R262 V265 P266 D267 S268 F269 L270 L280 K284 L297 L300 T328 D334 N357 I360 Y361 E362 K363 V364 R367 GLU
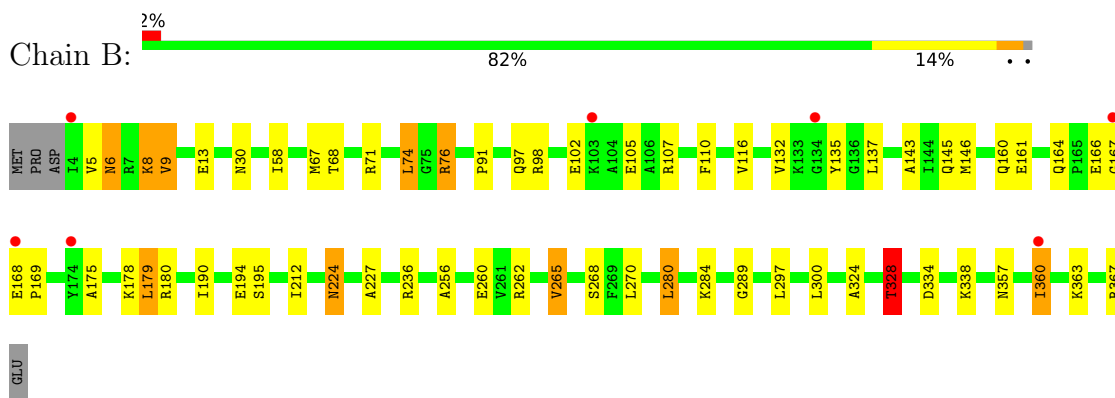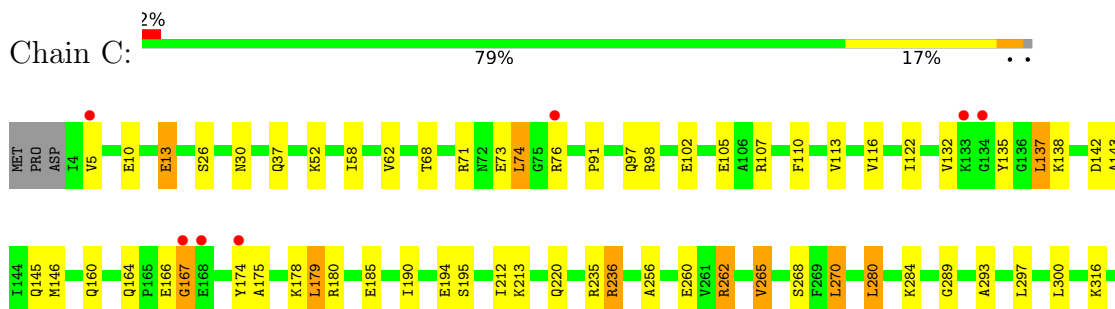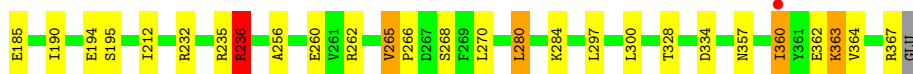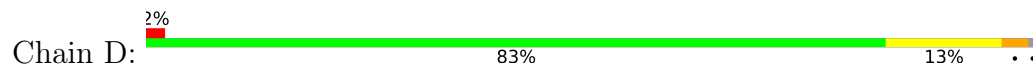
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.20Å　　101.20Å　　336.84Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	46.13　–　2.20 46.13　–　2.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.13-2.20) 95.6 (46.13-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.201　,　0.231 0.197　,　0.225	Depositor DCC
R_{free} test set	4303 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11968	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.73	3/2850 (0.1%)	0.88	11/3838 (0.3%)
1	B	0.73	1/2858 (0.0%)	0.81	7/3849 (0.2%)
1	C	0.73	3/2858 (0.1%)	0.89	14/3849 (0.4%)
1	D	0.74	3/2858 (0.1%)	0.91	12/3849 (0.3%)
All	All	0.74	10/11424 (0.1%)	0.87	44/15385 (0.3%)

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
1	C	0	1
1	D	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	262	ARG	CZ-NH2	-9.16	1.21	1.33
1	A	328	THR	CB-CG2	-8.90	1.23	1.52
1	B	328	THR	CB-CG2	-8.61	1.24	1.52
1	C	328	THR	CB-CG2	-6.74	1.30	1.52
1	D	328	THR	CB-CG2	-6.15	1.32	1.52
1	D	262	ARG	CZ-NH1	-5.80	1.25	1.33
1	C	37	GLN	CD-NE2	-5.59	1.18	1.32
1	A	270	LEU	CG-CD2	-5.52	1.31	1.51
1	A	270	LEU	CG-CD1	-5.31	1.32	1.51
1	C	37	GLN	CD-OE1	-5.18	1.12	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	236	ARG	NE-CZ-NH1	-17.51	111.55	120.30
1	D	236	ARG	NE-CZ-NH2	16.64	128.62	120.30
1	A	76	ARG	NE-CZ-NH1	-15.46	112.57	120.30
1	A	76	ARG	NE-CZ-NH2	14.97	127.78	120.30
1	C	98	ARG	NE-CZ-NH2	12.88	126.74	120.30
1	C	98	ARG	NE-CZ-NH1	-12.74	113.93	120.30
1	C	180	ARG	NE-CZ-NH1	-12.16	114.22	120.30
1	C	180	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	B	236	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	D	262	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	A	236	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	A	236	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	B	236	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	D	262	ARG	NE-CZ-NH2	8.89	124.75	120.30
1	D	262	ARG	NH1-CZ-NH2	-8.69	109.84	119.40
1	C	236	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	C	236	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	D	236	ARG	CD-NE-CZ	8.39	135.35	123.60
1	D	236	ARG	CG-CD-NE	8.10	128.80	111.80
1	A	76	ARG	CD-NE-CZ	7.50	134.10	123.60
1	A	270	LEU	CD1-CG-CD2	-7.06	89.33	110.50
1	B	180	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	D	76	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	D	180	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	C	76	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	76	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	D	236	ARG	CB-CG-CD	-5.96	96.11	111.60
1	B	180	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	365	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	76	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	180	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	262	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	A	328	THR	N-CA-CB	-5.62	99.62	110.30
1	A	98	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	236	ARG	CD-NE-CZ	5.45	131.22	123.60
1	C	236	ARG	CD-NE-CZ	5.41	131.17	123.60
1	B	236	ARG	CD-NE-CZ	5.38	131.13	123.60
1	D	76	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	180	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	76	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	328	THR	OG1-CB-CG2	-5.18	98.09	110.00
1	A	180	ARG	NE-CZ-NH2	-5.09	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	270	LEU	CB-CG-CD2	5.07	119.63	111.00
1	C	98	ARG	CD-NE-CZ	5.05	130.67	123.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	GLY	Peptide
1	B	167	GLY	Peptide
1	C	167	GLY	Peptide
1	D	167	GLY	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	2803	0	2888	47	0
1	B	2811	0	2899	44	0
1	C	2811	0	2899	47	0
1	D	2811	0	2899	40	0
2	A	46	0	30	9	0
2	B	46	0	30	9	0
2	C	46	0	30	8	0
2	D	46	0	30	8	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	124	0	0	7	0
4	B	138	0	0	8	0
4	C	146	0	0	5	0
4	D	137	0	0	5	0
All	All	11968	0	11705	183	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 8.

All (183) 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:30:ASN:HB3	4:B:487:HOH:O	1.22	1.32
1:D:161:GLU:HG3	4:D:516:HOH:O	1.32	1.26
1:C:160:GLN:OE1	2:C:669:VNR:H16B	1.43	1.16
1:A:160:GLN:OE1	2:A:669:VNR:H16B	1.47	1.13
1:D:160:GLN:OE1	2:D:669:VNR:H16B	1.49	1.12
1:B:195:SER:CB	2:B:669:VNR:H16	1.84	1.07
1:B:195:SER:HB2	2:B:669:VNR:H16	1.06	1.03
1:C:30:ASN:OD1	4:C:440:HOH:O	1.78	0.99
1:B:195:SER:HB2	2:B:669:VNR:C16	1.95	0.94
1:A:107:ARG:HA	1:A:146:MET:HE3	1.48	0.94
1:D:107:ARG:HA	1:D:146:MET:HE3	1.51	0.92
1:C:195:SER:HB2	2:C:669:VNR:H16	1.52	0.92
1:C:107:ARG:HA	1:C:146:MET:HE3	1.55	0.88
1:A:265:VAL:HG22	1:A:268:SER:HB3	1.60	0.83
1:A:195:SER:HB2	2:A:669:VNR:H16	1.61	0.83
1:B:107:ARG:HA	1:B:146:MET:HE3	1.59	0.83
1:D:265:VAL:HG22	1:D:268:SER:HB3	1.61	0.83
1:C:265:VAL:HG22	1:C:268:SER:HB3	1.60	0.83
1:B:265:VAL:HG22	1:B:268:SER:HB3	1.63	0.81
1:A:110:PHE:HB2	1:A:146:MET:HE2	1.63	0.80
1:C:195:SER:HB2	2:C:669:VNR:C16	2.11	0.80
1:D:195:SER:HB2	2:D:669:VNR:H16	1.63	0.80
1:A:195:SER:HB2	2:A:669:VNR:C16	2.14	0.78
1:B:160:GLN:OE1	2:B:669:VNR:H16B	1.84	0.77
1:B:338:LYS:NZ	4:B:493:HOH:O	2.09	0.77
1:D:195:SER:HB2	2:D:669:VNR:C16	2.15	0.76
1:C:362:GLU:O	1:C:366:LYS:HG2	1.86	0.75
1:B:195:SER:CB	2:B:669:VNR:C16	2.59	0.74
1:A:13:GLU:OE1	4:A:478:HOH:O	2.05	0.74
1:B:280:LEU:HD11	1:B:284:LYS:HE3	1.70	0.72
1:C:338:LYS:HB3	1:C:366:LYS:HB2	1.72	0.72
1:B:13:GLU:OE1	4:B:476:HOH:O	2.07	0.72
1:D:110:PHE:HB2	1:D:146:MET:HE2	1.72	0.71
1:C:280:LEU:O	1:C:280:LEU:HD12	1.91	0.71
1:A:280:LEU:HD12	1:A:280:LEU:O	1.92	0.69
1:B:5:VAL:CG1	1:B:71:ARG:HG3	2.22	0.69
1:D:5:VAL:HG13	1:D:71:ARG:HG3	1.75	0.68
1:D:280:LEU:HD11	1:D:284:LYS:HE3	1.76	0.67
1:B:324:ALA:O	1:B:328:THR:HB	1.94	0.67
1:B:161:GLU:OE1	4:B:401:HOH:O	2.12	0.66
1:C:110:PHE:HB2	1:C:146:MET:HE2	1.76	0.65
1:B:280:LEU:C	1:B:280:LEU:HD12	2.17	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ALA:O	1:A:328:THR:HB	1.98	0.63
1:B:97:GLN:NE2	1:B:143:ALA:HB1	2.14	0.62
1:C:97:GLN:NE2	1:C:143:ALA:HB1	2.13	0.62
2:B:669:VNR:H9	2:B:669:VNR:H2'	1.82	0.62
1:A:141:GLN:HG2	4:A:427:HOH:O	2.00	0.61
1:C:280:LEU:HD12	1:C:280:LEU:C	2.21	0.61
1:A:26:SER:H	1:A:220:GLN:HE21	1.47	0.61
1:A:110:PHE:CD1	1:A:146:MET:HE1	2.35	0.61
1:C:52:LYS:HG2	4:C:489:HOH:O	2.00	0.61
1:B:110:PHE:HB2	1:B:146:MET:HE2	1.81	0.61
4:B:482:HOH:O	1:C:316:LYS:HE3	2.01	0.60
1:D:180:ARG:HD2	4:D:378:HOH:O	2.00	0.60
1:D:280:LEU:HD12	1:D:280:LEU:C	2.21	0.60
1:A:195:SER:CB	2:A:669:VNR:C16	2.80	0.60
1:B:280:LEU:HD12	1:B:280:LEU:O	2.02	0.60
1:A:280:LEU:HD11	1:A:284:LYS:HE3	1.83	0.59
1:C:280:LEU:HD11	1:C:284:LYS:HE3	1.84	0.59
1:A:224:ASN:ND2	1:A:227:ALA:H	1.99	0.58
1:C:107:ARG:HA	1:C:146:MET:CE	2.31	0.58
1:B:5:VAL:HG12	1:B:71:ARG:HG3	1.86	0.58
1:C:110:PHE:CD1	1:C:146:MET:HE1	2.39	0.58
1:A:110:PHE:HB2	1:A:146:MET:CE	2.34	0.57
1:C:195:SER:CB	2:C:669:VNR:C16	2.82	0.57
1:B:110:PHE:CD1	1:B:146:MET:HE1	2.39	0.56
1:D:107:ARG:HA	1:D:146:MET:CE	2.32	0.56
1:B:107:ARG:HA	1:B:146:MET:CE	2.33	0.56
1:A:160:GLN:OE1	2:A:669:VNR:C16	2.38	0.56
1:B:107:ARG:HD3	4:B:512:HOH:O	2.05	0.56
1:D:195:SER:CB	2:D:669:VNR:C16	2.85	0.55
1:D:13:GLU:HG2	4:D:377:HOH:O	2.05	0.55
1:D:185:GLU:OE1	4:D:406:HOH:O	2.18	0.55
1:C:132:VAL:CG1	1:C:175:ALA:HB2	2.36	0.54
1:D:110:PHE:CD1	1:D:146:MET:HE1	2.41	0.54
1:A:107:ARG:CA	1:A:146:MET:HE3	2.32	0.54
1:C:135:TYR:O	1:C:178:LYS:HE2	2.07	0.54
1:D:68:THR:OG1	1:D:74:LEU:HG	2.08	0.54
1:A:280:LEU:HD12	1:A:280:LEU:C	2.28	0.54
1:B:135:TYR:O	1:B:178:LYS:HE2	2.07	0.54
1:D:160:GLN:OE1	2:D:669:VNR:C16	2.41	0.53
1:D:280:LEU:HD12	1:D:280:LEU:O	2.08	0.53
1:A:195:SER:CB	2:A:669:VNR:H16A	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ASN:C	1:B:224:ASN:HD22	2.10	0.53
1:A:366:LYS:NZ	4:A:394:HOH:O	2.43	0.52
1:C:174:TYR:HB3	4:C:439:HOH:O	2.09	0.52
1:B:68:THR:OG1	1:B:74:LEU:HG	2.11	0.51
1:D:132:VAL:HG13	1:D:175:ALA:HB2	1.93	0.51
1:B:280:LEU:C	1:B:280:LEU:CD1	2.77	0.51
1:C:137:LEU:HD21	1:C:185:GLU:HB2	1.92	0.51
1:D:232:ARG:O	1:D:236:ARG:HG2	2.11	0.51
1:C:68:THR:OG1	1:C:74:LEU:HG	2.11	0.51
1:C:357:ASN:OD1	1:C:360:ILE:HG23	2.10	0.51
1:C:179:LEU:HD22	1:C:190:ILE:HD13	1.93	0.50
1:A:107:ARG:HA	1:A:146:MET:CE	2.31	0.50
1:B:132:VAL:CG1	1:B:175:ALA:HB2	2.42	0.50
1:B:6:ASN:HA	1:B:9:VAL:HG13	1.93	0.49
1:B:67:MET:HA	2:B:669:VNR:N5	2.28	0.49
1:D:256:ALA:O	1:D:260:GLU:HG3	2.11	0.49
1:D:363:LYS:HE3	1:D:363:LYS:HA	1.94	0.49
1:D:195:SER:CB	2:D:669:VNR:H16A	2.42	0.49
1:C:235:ARG:HD2	4:C:430:HOH:O	2.12	0.49
1:D:13:GLU:CG	4:D:377:HOH:O	2.60	0.49
1:D:58:ILE:HG21	1:D:91:PRO:HG3	1.94	0.49
1:A:328:THR:HG22	1:A:330:SER:OG	2.12	0.49
1:A:68:THR:OG1	1:A:74:LEU:HG	2.13	0.48
1:C:5:VAL:HG13	1:C:71:ARG:HG3	1.95	0.48
1:B:256:ALA:O	1:B:260:GLU:HG3	2.13	0.48
1:A:224:ASN:C	1:A:224:ASN:HD22	2.16	0.48
1:A:195:SER:CB	2:A:669:VNR:H16	2.39	0.48
1:C:195:SER:CB	2:C:669:VNR:H16A	2.43	0.48
1:D:280:LEU:C	1:D:280:LEU:CD1	2.82	0.48
1:D:357:ASN:OD1	1:D:360:ILE:HG23	2.14	0.47
1:B:280:LEU:O	1:B:280:LEU:CD1	2.62	0.47
1:A:13:GLU:HG2	4:A:422:HOH:O	2.14	0.47
1:D:179:LEU:HD13	1:D:212:ILE:HD11	1.97	0.47
1:B:169:PRO:HA	4:B:401:HOH:O	2.15	0.46
1:A:168:GLU:O	4:A:468:HOH:O	2.20	0.46
2:B:669:VNR:H11A	2:B:669:VNR:H12A	1.62	0.46
1:D:5:VAL:O	1:D:8:LYS:HB2	2.16	0.46
1:D:132:VAL:CG1	1:D:175:ALA:HB2	2.45	0.46
1:C:132:VAL:HG13	1:C:175:ALA:HB2	1.98	0.46
1:C:110:PHE:HB2	1:C:146:MET:CE	2.44	0.46
1:B:179:LEU:HD22	1:B:190:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:VAL:CG1	1:D:71:ARG:HG3	2.45	0.46
1:A:179:LEU:HD22	1:A:190:ILE:HD13	1.97	0.45
1:B:168:GLU:HA	1:B:169:PRO:HD3	1.73	0.45
1:C:256:ALA:O	1:C:260:GLU:HG3	2.16	0.45
1:A:83:GLU:HB3	1:A:116:VAL:HG13	1.97	0.45
1:B:58:ILE:HG21	1:B:91:PRO:HG3	1.97	0.45
1:C:58:ILE:HG21	1:C:91:PRO:HG3	1.98	0.45
1:C:97:GLN:HE22	1:C:143:ALA:HB1	1.81	0.45
2:A:669:VNR:H11A	2:A:669:VNR:H12A	1.51	0.45
1:C:353:TYR:OH	1:D:362:GLU:OE1	2.28	0.45
1:B:179:LEU:HD13	1:B:212:ILE:HD11	1.99	0.44
1:C:262:ARG:HD2	1:C:289:GLY:O	2.18	0.44
2:C:669:VNR:H9	2:C:669:VNR:H2'	1.99	0.44
2:C:669:VNR:H11A	2:C:669:VNR:H12A	1.70	0.44
1:A:256:ALA:O	1:A:260:GLU:HG3	2.17	0.44
1:C:26:SER:H	1:C:220:GLN:HE21	1.65	0.44
1:B:5:VAL:O	1:B:8:LYS:HB2	2.18	0.43
1:D:110:PHE:HB2	1:D:146:MET:CE	2.43	0.43
1:A:205:LYS:HE3	1:A:264:SER:HB2	2.00	0.43
1:D:179:LEU:HD22	1:D:190:ILE:HD13	1.99	0.43
1:A:261:VAL:CG1	1:A:270:LEU:HD12	2.49	0.43
1:A:168:GLU:HA	1:A:169:PRO:HD3	1.73	0.43
1:A:328:THR:HG23	1:A:339:THR:OG1	2.18	0.43
1:D:73:GLU:H	1:D:73:GLU:CD	2.22	0.43
1:A:357:ASN:OD1	1:A:360:ILE:HG23	2.19	0.43
1:A:62:VAL:HA	1:A:293:ALA:O	2.19	0.42
1:C:113:VAL:CG1	1:C:122:ILE:HD12	2.49	0.42
1:C:179:LEU:HD13	1:C:212:ILE:HD11	2.00	0.42
1:C:213:LYS:NZ	4:C:419:HOH:O	2.52	0.42
1:C:13:GLU:OE2	1:C:235:ARG:NH2	2.52	0.42
1:C:195:SER:CB	2:C:669:VNR:H16	2.37	0.42
1:D:266:PRO:HB3	1:D:364:VAL:HG13	2.01	0.42
1:C:73:GLU:H	1:C:73:GLU:CD	2.22	0.42
1:C:363:LYS:O	1:C:367:ARG:HG2	2.20	0.42
1:A:138:LYS:HE2	1:A:142:ASP:OD2	2.19	0.42
1:A:180:ARG:HD2	4:A:424:HOH:O	2.20	0.42
1:A:7:ARG:NH1	2:A:669:VNR:O88	2.53	0.41
1:B:367:ARG:CZ	4:B:467:HOH:O	2.67	0.41
1:D:67:MET:HA	2:D:669:VNR:N5	2.35	0.41
1:B:262:ARG:HD2	1:B:289:GLY:O	2.20	0.41
2:D:669:VNR:H12A	2:D:669:VNR:H11A	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:O	1:A:178:LYS:HE2	2.20	0.41
1:A:179:LEU:HD13	1:A:212:ILE:HD11	2.03	0.41
1:C:338:LYS:HE3	1:C:366:LYS:O	2.20	0.41
1:B:224:ASN:ND2	1:B:227:ALA:H	2.18	0.41
1:B:5:VAL:HG11	1:B:71:ARG:HG3	1.98	0.41
1:B:280:LEU:CD1	1:B:284:LYS:HE3	2.46	0.41
1:A:13:GLU:CG	4:A:422:HOH:O	2.69	0.41
1:A:132:VAL:CG1	1:A:175:ALA:HB2	2.51	0.41
1:C:138:LYS:HE2	1:C:142:ASP:OD2	2.21	0.41
1:D:168:GLU:HA	1:D:169:PRO:HD3	1.72	0.41
1:A:363:LYS:HE3	1:A:363:LYS:N	2.36	0.41
1:B:8:LYS:NZ	2:B:669:VNR:O22	2.54	0.41
1:C:10:GLU:CD	1:C:236:ARG:HH22	2.24	0.41
1:C:62:VAL:HA	1:C:293:ALA:O	2.20	0.41
1:D:13:GLU:OE2	1:D:235:ARG:NH2	2.52	0.41
1:A:132:VAL:HG13	1:A:175:ALA:HB2	2.03	0.41
1:A:217:THR:O	1:A:218:SER:C	2.59	0.40
1:B:357:ASN:OD1	1:B:360:ILE:HG23	2.21	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	361/368 (98%)	350 (97%)	10 (3%)	1 (0%)	41	46
1	B	362/368 (98%)	351 (97%)	10 (3%)	1 (0%)	41	46
1	C	362/368 (98%)	347 (96%)	13 (4%)	2 (1%)	25	26
1	D	362/368 (98%)	350 (97%)	11 (3%)	1 (0%)	41	46
All	All	1447/1472 (98%)	1398 (97%)	44 (3%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	GLU
1	B	102	GLU
1	C	102	GLU
1	C	167	GLY
1	D	102	GLU

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	297/302 (98%)	274 (92%)	23 (8%)	13	13
1	B	298/302 (99%)	274 (92%)	24 (8%)	11	12
1	C	298/302 (99%)	280 (94%)	18 (6%)	19	22
1	D	298/302 (99%)	273 (92%)	25 (8%)	11	11
All	All	1191/1208 (99%)	1101 (92%)	90 (8%)	13	14

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	8	LYS
1	A	74	LEU
1	A	98	ARG
1	A	105	GLU
1	A	116	VAL
1	A	137	LEU
1	A	145	GLN
1	A	161	GLU
1	A	164	GLN
1	A	166	GLU
1	A	179	LEU
1	A	194	GLU
1	A	224	ASN
1	A	265	VAL
1	A	280	LEU
1	A	297	LEU

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Mol	Chain	Res	Type
1	A	300	LEU
1	A	328	THR
1	A	334	ASP
1	A	360	ILE
1	A	363	LYS
1	A	367	ARG
1	B	6	ASN
1	B	8	LYS
1	B	9	VAL
1	B	74	LEU
1	B	76	ARG
1	B	98	ARG
1	B	105	GLU
1	B	116	VAL
1	B	137	LEU
1	B	145	GLN
1	B	164	GLN
1	B	166	GLU
1	B	179	LEU
1	B	194	GLU
1	B	224	ASN
1	B	265	VAL
1	B	270	LEU
1	B	280	LEU
1	B	297	LEU
1	B	300	LEU
1	B	328	THR
1	B	334	ASP
1	B	360	ILE
1	B	363	LYS
1	C	13	GLU
1	C	74	LEU
1	C	105	GLU
1	C	116	VAL
1	C	137	LEU
1	C	145	GLN
1	C	164	GLN
1	C	166	GLU
1	C	179	LEU
1	C	194	GLU
1	C	265	VAL
1	C	270	LEU

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Mol	Chain	Res	Type
1	C	280	LEU
1	C	297	LEU
1	C	300	LEU
1	C	334	ASP
1	C	360	ILE
1	C	363	LYS
1	D	4	ILE
1	D	6	ASN
1	D	8	LYS
1	D	13	GLU
1	D	74	LEU
1	D	76	ARG
1	D	98	ARG
1	D	105	GLU
1	D	116	VAL
1	D	137	LEU
1	D	145	GLN
1	D	164	GLN
1	D	166	GLU
1	D	179	LEU
1	D	194	GLU
1	D	236	ARG
1	D	265	VAL
1	D	270	LEU
1	D	280	LEU
1	D	297	LEU
1	D	300	LEU
1	D	334	ASP
1	D	360	ILE
1	D	363	LYS
1	D	367	ARG

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

Mol	Chain	Res	Type
1	A	145	GLN
1	A	197	ASN
1	A	220	GLN
1	A	224	ASN
1	B	97	GLN
1	B	145	GLN
1	B	197	ASN

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Mol	Chain	Res	Type
1	B	224	ASN
1	C	37	GLN
1	C	97	GLN
1	C	145	GLN
1	C	197	ASN
1	C	220	GLN
1	D	145	GLN
1	D	197	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	VNR	B	669	-	45,48,48	1.70	6 (13%)	56,74,74	1.36	5 (8%)
2	VNR	A	669	3	45,48,48	1.74	8 (17%)	56,74,74	1.66	7 (12%)
2	VNR	D	669	3	45,48,48	1.64	7 (15%)	56,74,74	1.46	9 (16%)
2	VNR	C	669	3	45,48,48	1.69	4 (8%)	56,74,74	1.85	9 (16%)

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	VNR	B	669	-	-	11/38/71/71	0/3/3/3
2	VNR	A	669	3	-	12/38/71/71	0/3/3/3
2	VNR	D	669	3	-	10/38/71/71	0/3/3/3
2	VNR	C	669	3	-	10/38/71/71	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	669	VNR	C5A-C9A	7.95	1.49	1.40
2	A	669	VNR	C5A-C9A	7.80	1.49	1.40
2	D	669	VNR	C5A-C9A	7.49	1.49	1.40
2	B	669	VNR	C5A-C9A	6.50	1.48	1.40
2	B	669	VNR	C4A-C4	-4.53	1.49	1.54
2	C	669	VNR	C4A-C4	-3.84	1.50	1.54
2	C	669	VNR	C8-C7	3.68	1.50	1.40
2	B	669	VNR	C5A-N5	-3.68	1.33	1.38
2	D	669	VNR	C4A-C4	-3.39	1.51	1.54
2	B	669	VNR	C8-C7	3.38	1.49	1.40
2	A	669	VNR	C5A-N5	-3.36	1.33	1.38
2	D	669	VNR	C8-C7	3.19	1.48	1.40
2	A	669	VNR	C11-C14	-3.17	1.47	1.51
2	B	669	VNR	C4A-N5	-3.15	1.43	1.46
2	C	669	VNR	C5A-N5	-3.15	1.33	1.38
2	A	669	VNR	C4A-C4	-3.03	1.51	1.54
2	A	669	VNR	C8-C7	3.03	1.48	1.40
2	A	669	VNR	C11-C4A	-2.64	1.51	1.55
2	A	669	VNR	O4-C4	2.61	1.27	1.22
2	D	669	VNR	C4A-N5	-2.60	1.44	1.46
2	D	669	VNR	C11-C4A	-2.51	1.52	1.55
2	D	669	VNR	C11-C14	-2.37	1.48	1.51
2	B	669	VNR	C5'-C4'	2.34	1.55	1.51
2	D	669	VNR	C5A-N5	-2.29	1.35	1.38
2	A	669	VNR	C4A-N5	-2.13	1.44	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	669	VNR	O4-C4-C4A	-9.36	116.97	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	669	VNR	O4-C4-C4A	-7.61	118.40	124.61
2	B	669	VNR	O4-C4-C4A	-6.54	119.27	124.61
2	D	669	VNR	C10-C4A-N5	4.53	110.97	106.29
2	A	669	VNR	C10-C4A-N5	4.51	110.94	106.29
2	D	669	VNR	O4-C4-C4A	-4.06	121.30	124.61
2	C	669	VNR	C4-N3-C2	-3.79	119.70	125.42
2	C	669	VNR	C9A-C5A-N5	-3.74	114.99	119.19
2	A	669	VNR	C16-C15-C14	-3.65	120.26	127.19
2	D	669	VNR	C16-C15-C14	-3.52	120.50	127.19
2	C	669	VNR	C10-C4A-N5	3.51	109.92	106.29
2	D	669	VNR	C4-N3-C2	-2.79	121.22	125.42
2	C	669	VNR	C16-C15-C14	-2.78	121.91	127.19
2	C	669	VNR	C4A-C4-N3	2.70	120.25	117.16
2	A	669	VNR	O2-C2-N1	-2.70	117.36	121.83
2	B	669	VNR	C16-C15-C14	-2.69	122.07	127.19
2	B	669	VNR	C9A-C5A-N5	-2.68	116.17	119.19
2	A	669	VNR	C4-N3-C2	-2.58	121.53	125.42
2	D	669	VNR	P99-O66-P55	-2.58	123.99	132.83
2	D	669	VNR	O2-C2-N1	-2.50	117.68	121.83
2	B	669	VNR	C4-N3-C2	-2.47	121.70	125.42
2	A	669	VNR	P99-O66-P55	-2.33	124.82	132.83
2	D	669	VNR	O5'-P-O3P	-2.28	100.07	106.47
2	C	669	VNR	O2-C2-N1	-2.28	118.05	121.83
2	A	669	VNR	O2P-P-O1P	2.27	116.30	107.64
2	D	669	VNR	C9A-C5A-N5	-2.23	116.68	119.19
2	B	669	VNR	O2-C2-N1	-2.21	118.17	121.83
2	C	669	VNR	P99-O66-P55	-2.16	125.40	132.83
2	D	669	VNR	C4A-C4-N3	2.15	119.61	117.16
2	C	669	VNR	O44-P55-O33	2.12	115.75	107.64

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	669	VNR	C14-C11-C4A-N5
2	A	669	VNR	O15-C12-C13-C14
2	A	669	VNR	C12-O15-P99-O66
2	A	669	VNR	P99-O66-P55-O33
2	A	669	VNR	P99-O66-P55-O44
2	B	669	VNR	C14-C11-C4A-N5
2	B	669	VNR	O15-C12-C13-C14
2	B	669	VNR	C12-C13-C14-C11

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Mol	Chain	Res	Type	Atoms
2	B	669	VNR	C12-C13-C14-C15
2	B	669	VNR	C12-O15-P99-O66
2	B	669	VNR	C12-O15-P99-O77
2	C	669	VNR	C14-C11-C4A-N5
2	C	669	VNR	O15-C12-C13-C14
2	C	669	VNR	C12-O15-P99-O66
2	C	669	VNR	C12-O15-P99-O88
2	D	669	VNR	C14-C11-C4A-N5
2	D	669	VNR	O15-C12-C13-C14
2	D	669	VNR	C12-O15-P99-O66
2	D	669	VNR	C12-O15-P99-O88
2	B	669	VNR	C2'-C1'-N10-C10
2	C	669	VNR	C2'-C1'-N10-C10
2	A	669	VNR	C2'-C3'-C4'-O4'
2	C	669	VNR	C2'-C3'-C4'-O4'
2	B	669	VNR	C2'-C3'-C4'-O4'
2	B	669	VNR	C4'-C5'-O5'-P
2	A	669	VNR	C4'-C5'-O5'-P
2	C	669	VNR	C4'-C5'-O5'-P
2	D	669	VNR	C4'-C5'-O5'-P
2	A	669	VNR	C12-O15-P99-O77
2	A	669	VNR	C12-O15-P99-O88
2	B	669	VNR	C12-O15-P99-O88
2	C	669	VNR	C12-O15-P99-O77
2	D	669	VNR	C12-O15-P99-O77
2	A	669	VNR	O3'-C3'-C4'-O4'
2	D	669	VNR	C2'-C3'-C4'-O4'
2	A	669	VNR	O3'-C3'-C4'-C5'
2	D	669	VNR	O3'-C3'-C4'-O4'
2	C	669	VNR	O3'-C3'-C4'-O4'
2	D	669	VNR	O3'-C3'-C4'-C5'
2	A	669	VNR	P99-O66-P55-O22
2	B	669	VNR	O3'-C3'-C4'-O4'
2	C	669	VNR	C12-C13-C14-C11
2	D	669	VNR	C12-C13-C14-C11

There are no ring outliers.

4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	669	VNR	9	0
2	A	669	VNR	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	669	VNR	8	0
2	C	669	VNR	8	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 VNR B 669

Bond lengths

Bond angles

Torsions

Rings

Ligand VNR A 669

Bond lengths

Bond angles

Torsions

Rings

Ligand VNR D 669

Bond lengths

Bond angles

Torsions

Rings

Ligand VNR C 669

Bond lengths

Bond angles

Torsions

Rings
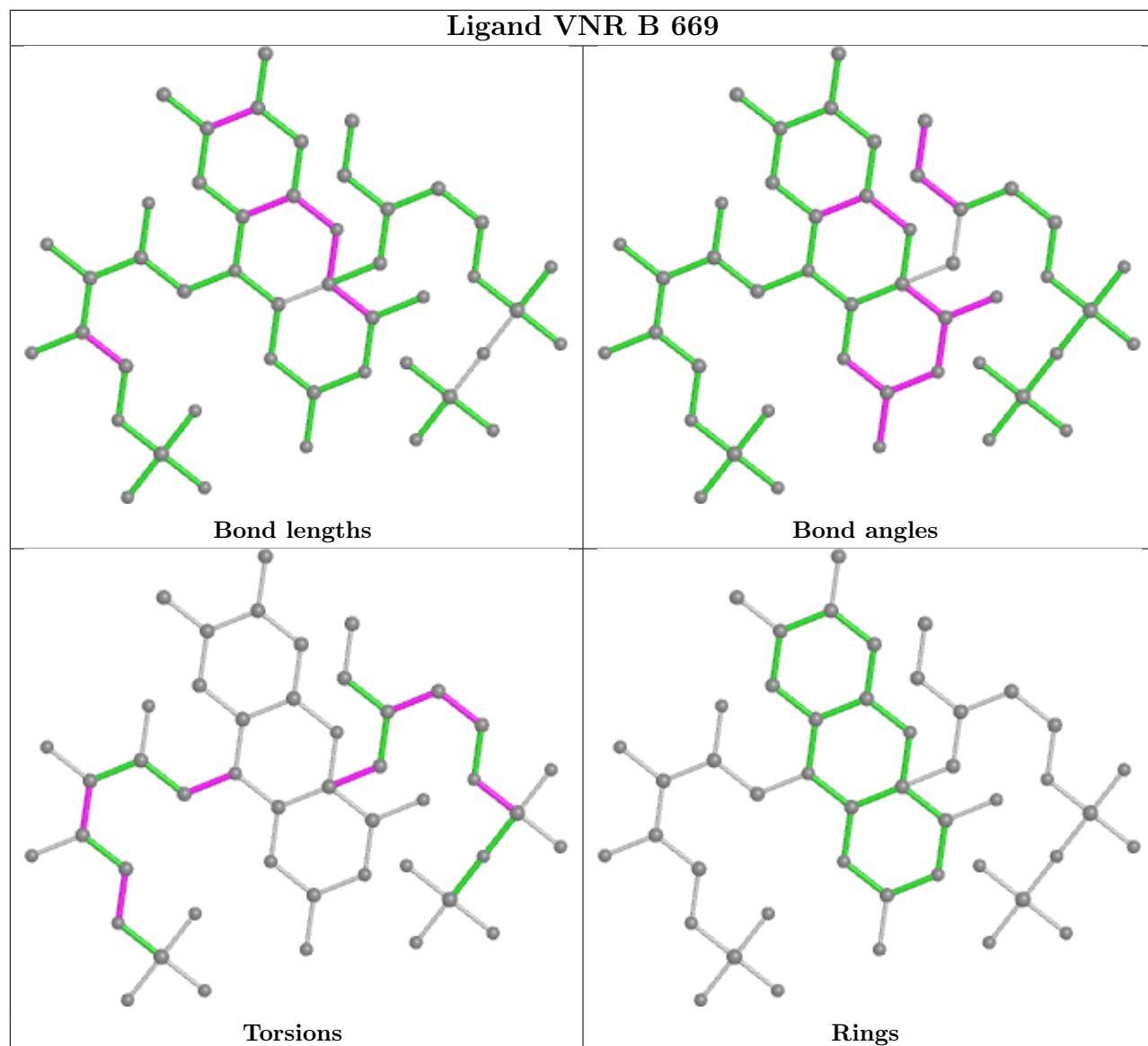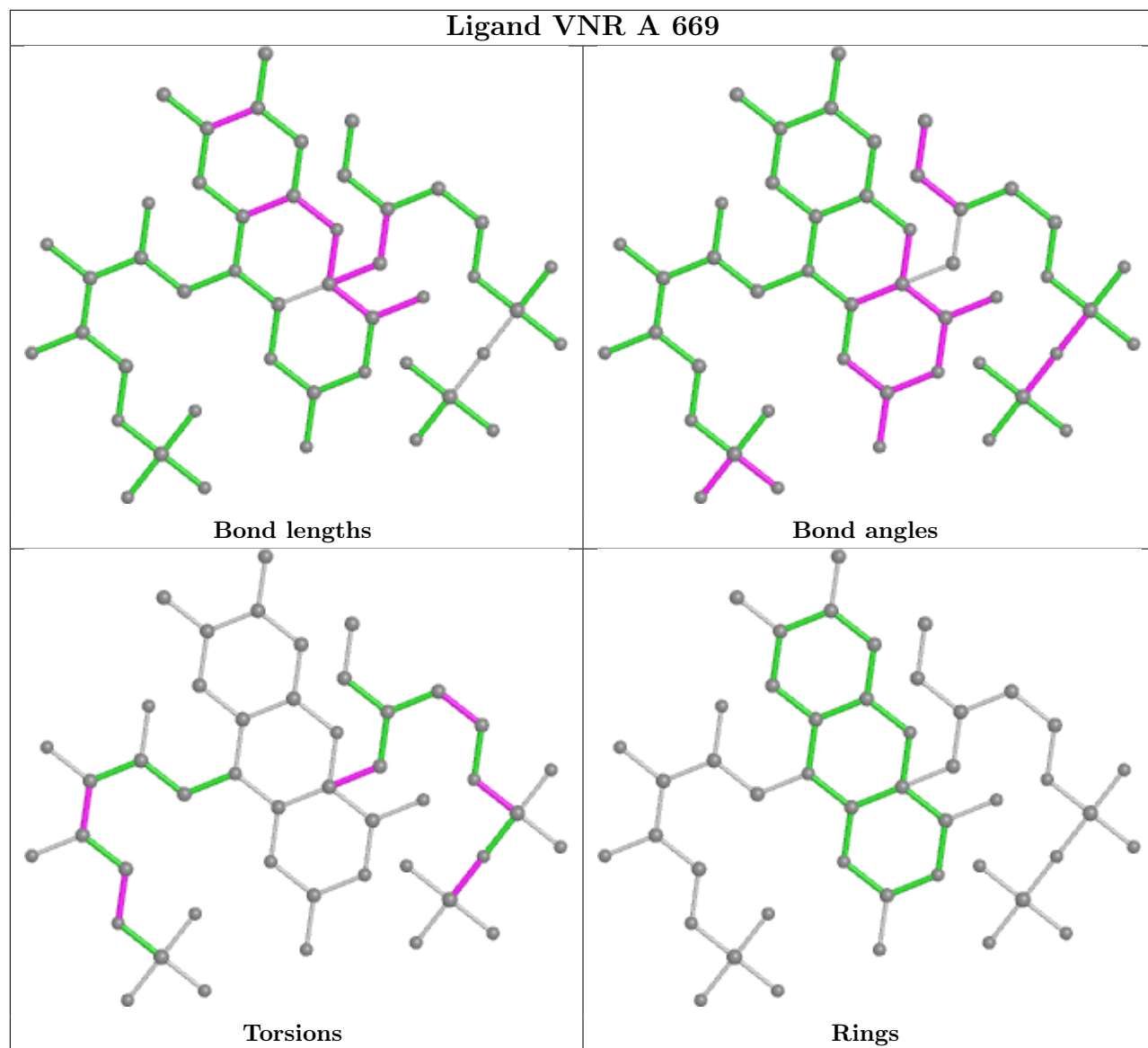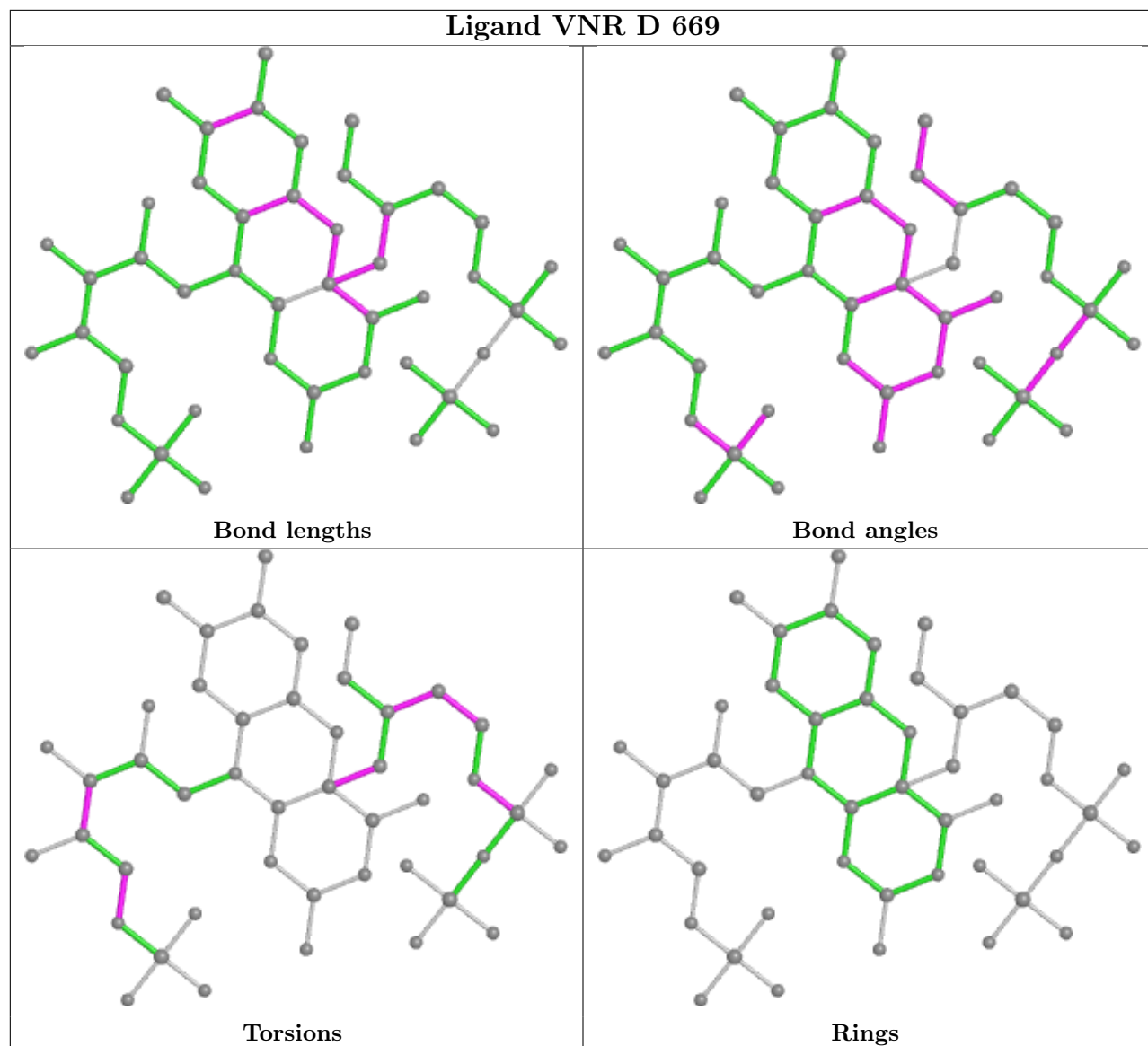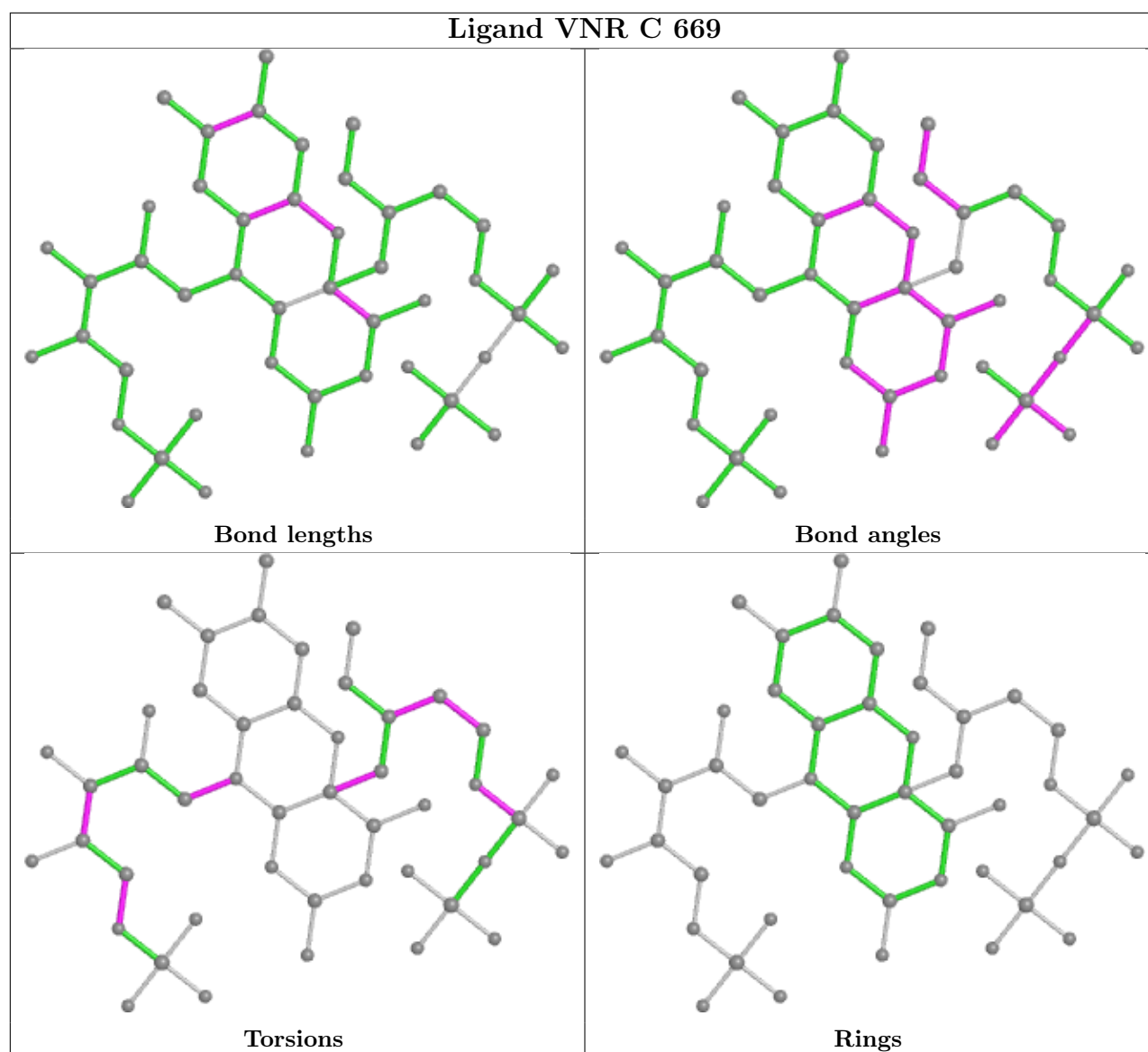
5.7 Other polymers ⓘ

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, 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	363/368 (98%)	-0.38	6 (1%)	70	68	23, 33, 53, 66	0
1	B	364/368 (98%)	-0.34	7 (1%)	66	65	23, 33, 55, 66	0
1	C	364/368 (98%)	-0.36	8 (2%)	62	59	23, 33, 54, 66	0
1	D	364/368 (98%)	-0.40	6 (1%)	72	70	24, 33, 54, 66	0
All	All	1455/1472 (98%)	-0.37	27 (1%)	66	65	23, 33, 55, 66	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	GLU	5.2
1	C	167	GLY	5.2
1	C	168	GLU	4.7
1	A	168	GLU	4.3
1	D	167	GLY	4.1
1	B	167	GLY	4.1
1	A	167	GLY	4.0
1	B	174	TYR	3.8
1	D	4	ILE	3.7
1	C	5	VAL	3.4
1	C	134	GLY	3.4
1	C	174	TYR	3.4
1	D	168	GLU	3.2
1	A	166	GLU	3.2
1	D	5	VAL	3.0
1	C	76	ARG	3.0
1	D	103	LYS	2.9
1	B	360	ILE	2.7
1	C	133	LYS	2.6
1	A	5	VAL	2.5
1	B	134	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	357	ASN	2.3
1	D	360	ILE	2.3
1	B	103	LYS	2.3
1	B	4	ILE	2.2
1	A	103	LYS	2.1
1	A	239	TRP	2.1

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 monosaccharides 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. 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
3	MG	D	1001	1/1	0.80	0.06	69,69,69,69	0
3	MG	A	1001	1/1	0.83	0.09	63,63,63,63	0
3	MG	C	1001	1/1	0.90	0.14	64,64,64,64	0
2	VNR	A	669	46/46	0.96	0.10	21,30,54,57	0
2	VNR	B	669	46/46	0.96	0.10	23,31,63,64	0
2	VNR	D	669	46/46	0.96	0.10	24,32,55,56	0
2	VNR	C	669	46/46	0.97	0.09	25,32,53,55	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 VNR A 669:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
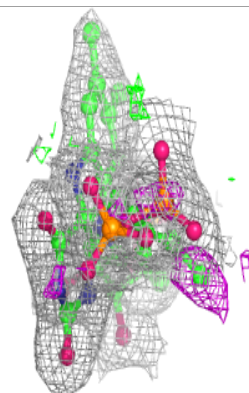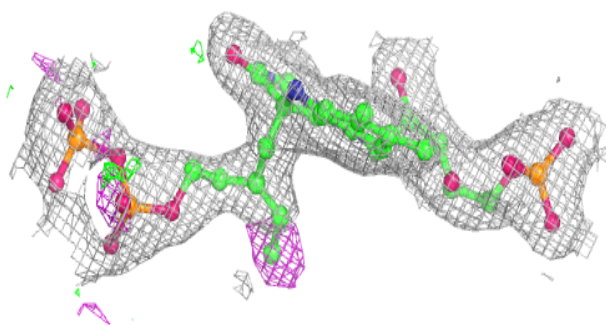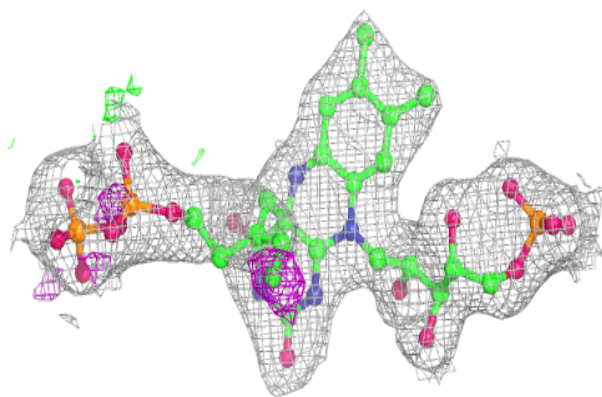and green (positive)
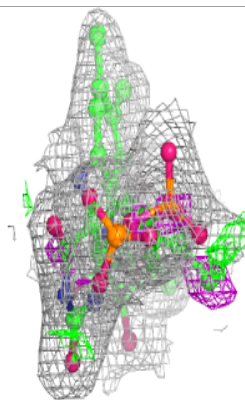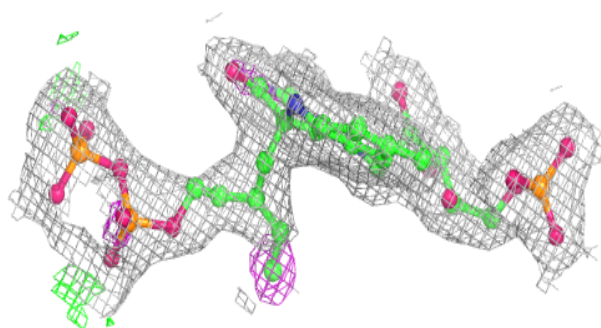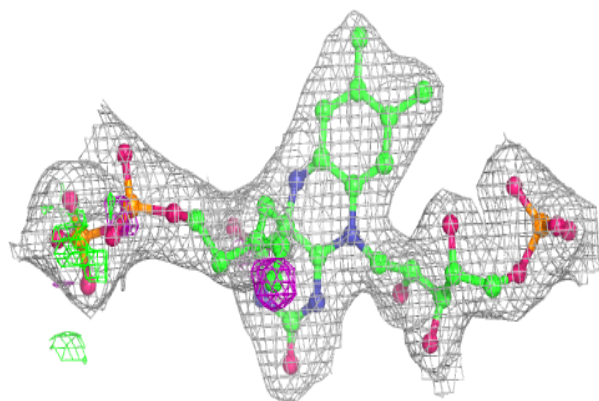
Electron density around VNR B 669:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
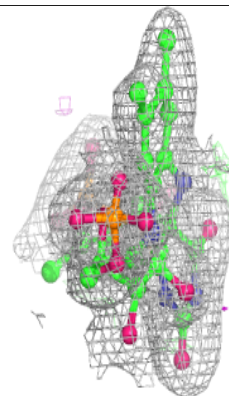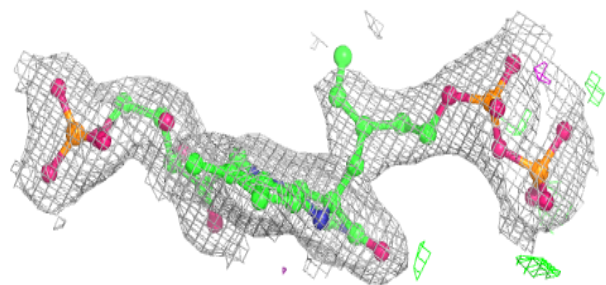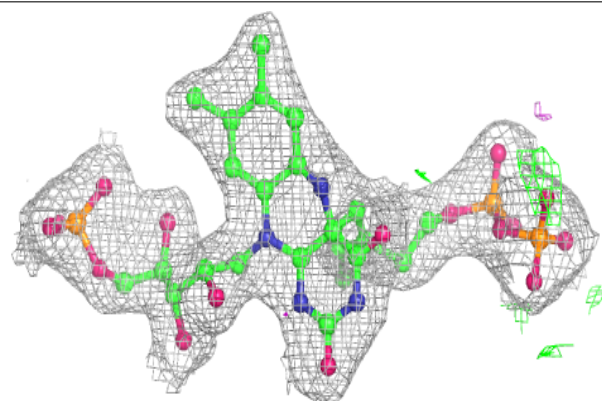and green (positive)
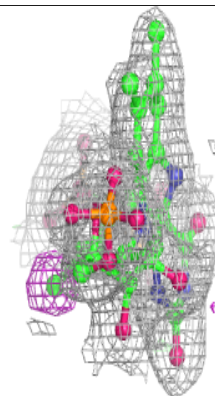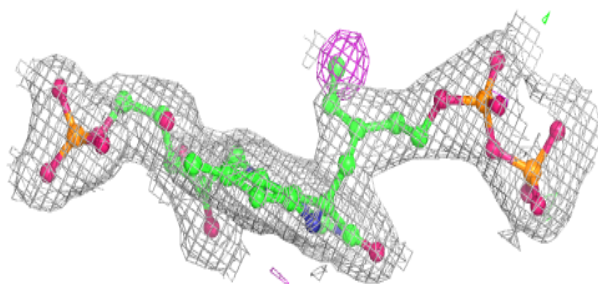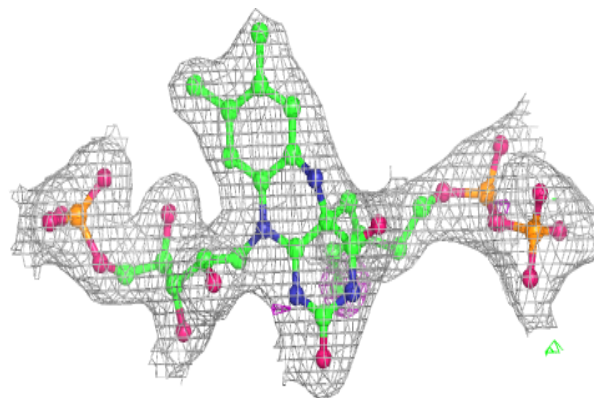
Electron density around VNR D 669:

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

Electron density around VNR C 669:

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

6.5 Other polymers (i)

There are no such residues in this entry.