Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2026 – 07:59 am BST

PDB ID	:	6YSO / pdb_00006yso
Title	:	Crystal structure of the (SR) Ca2+-ATPase solved by vanadium SAD phasing
Authors	:	El Omari, K.; Mohamad, N.; Bountra, K.; Duman, R.; Romano, M.; Schlegel, K.; Kwong, H.; Mykhaylyk, V.; Olesen, C.E.; Moller, J.V.; Bublitz, M.; Beis, K.; Wagner, A.
Deposited on	:	2020-04-22
Resolution	:	3.13 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:

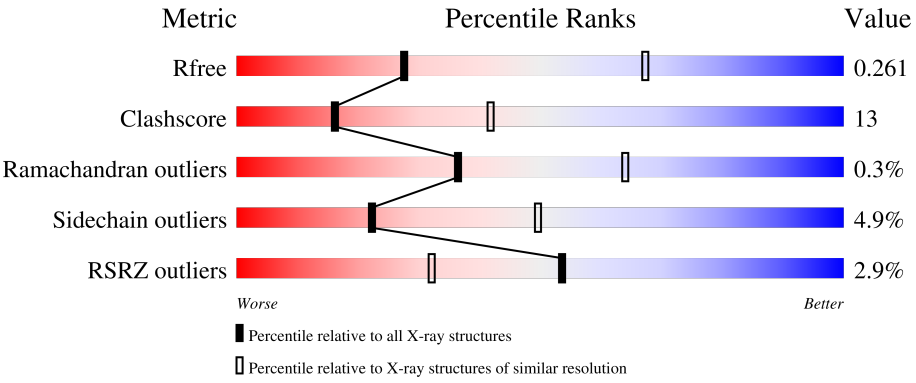
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.13 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	994	2% 69% 28%
1	B	994	4% 71% 26%

2 Entry composition

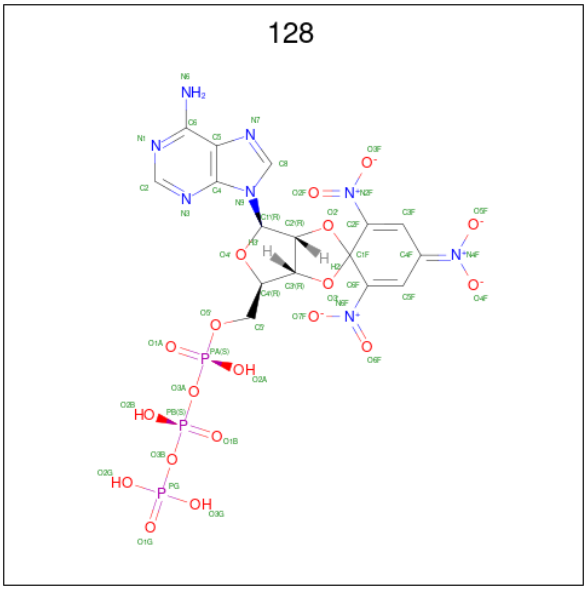
There are 8 unique types of molecules in this entry. The entry contains 15376 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	982	Total	C	N	O	S	0	0	0
			7569	4816	1268	1428	57			
1	B	985	Total	C	N	O	S	0	0	0
			7599	4833	1275	1434	57			

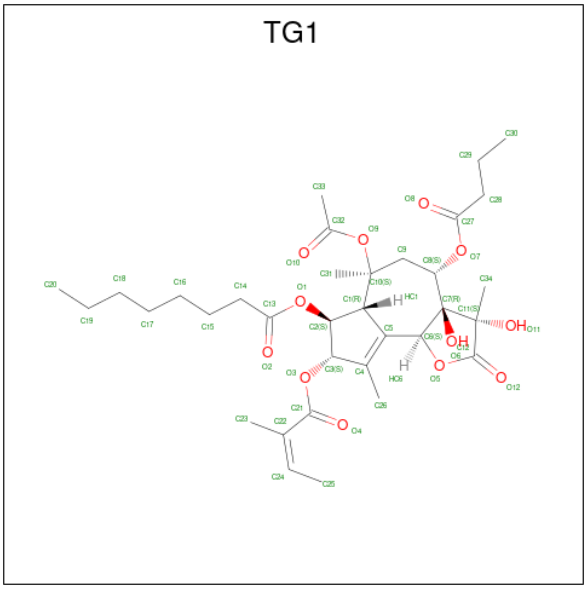
- Molecule 2 is SPIRO(2,4,6-TRINITROBENZENE[1,2A]-2O',3O'-METHYLENE-ADENINE-TRIPHOSPHATE (CCD ID: 128) (formula: $C_{16}H_{16}N_8O_{19}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			46	16	8	19	3		
2	B	1	Total	C	N	O	P	0	0
			46	16	8	19	3		

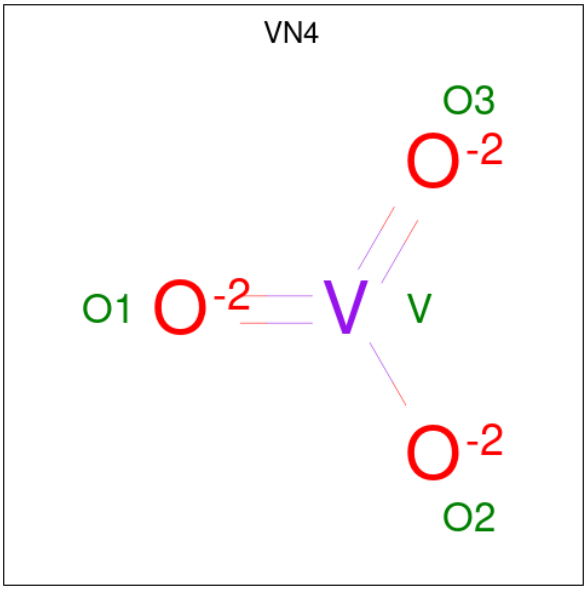
- Molecule 3 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OX

Y]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (CCD ID: TG1) (formula: $C_{34}H_{50}O_{12}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 46 34 12	0	0
3	B	1	Total C O 46 34 12	0	0

- Molecule 4 is oxido(dioxo)vanadium (CCD ID: VN4) (formula: O_3V) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O V 4 3 1	0	0
4	B	1	Total O V 4 3 1	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	B	2	Total Mg 2 2	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0
7	B	1	Total K 1 1	0	0

- Molecule 8 is water.

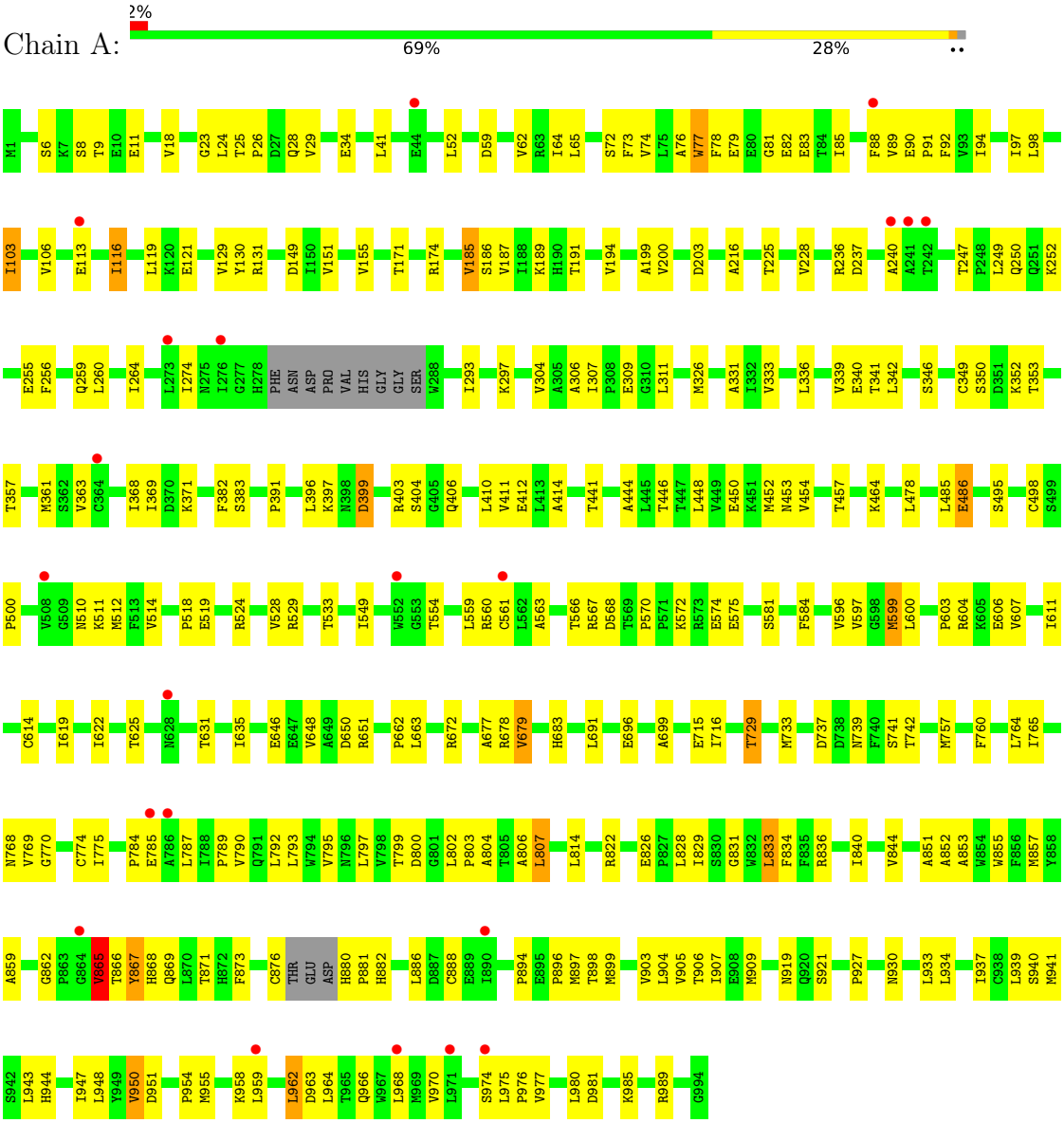
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	4	Total O 4 4	0	0
8	B	4	Total O 4 4	0	0

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: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

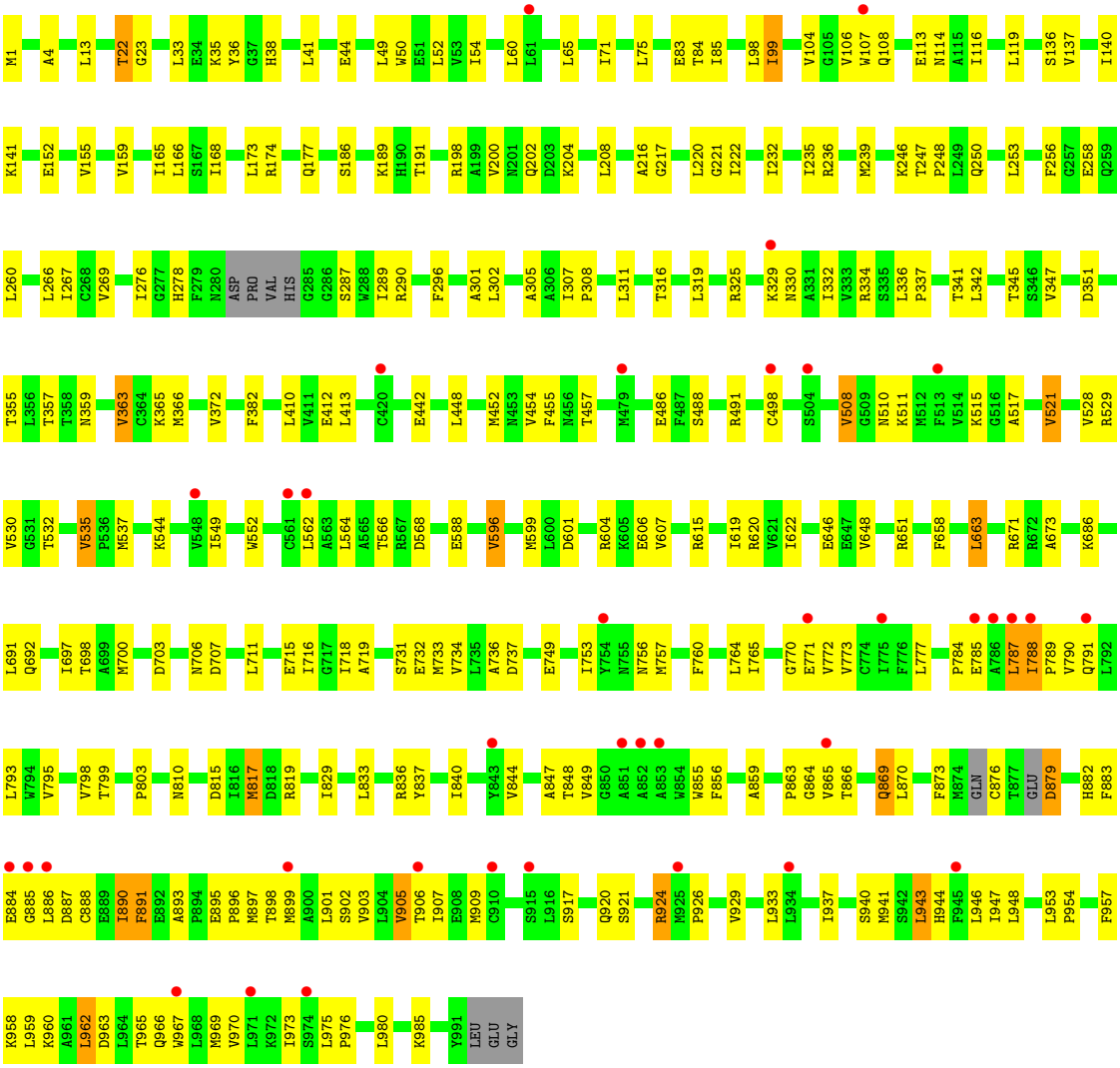
Chain A:



• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain B:




M1 A4 L13 T22 G23 L33 E34 K35 Y36 G37 H38 L41 E44 L49 W50 E51 L52 V53 I54 L60 L61 L65 I71 L75 E83 T84 I85 L98 I99 V104 G105 V106 W107 Q108 E113 N114 A115 I116 L119 S136 V137 I140
K141 E152 V155 V159 I165 L166 S167 I168 L173 R174 Q177 S186 K189 H190 T191 R198 A199 V200 N201 Q202 D203 K204 L208 A216 G217 L220 G221 I222 I232 I235 R236 M239 K246 T247 P248 L249 Q250 L253 F256 G257 E258 Q259
L260 L266 I267 C268 V269 I276 G277 H278 F279 N280 ASP PRO VAL HIS G285 G286 S287 W288 I289 R290 F296 A301 L302 A305 A306 I307 P308 L311 T316 L319 R325 K329 N330 A331 I332 V333 R334 S335 L336 P337 T341 L342 T345 S346 V347 D351
T355 L356 T357 T358 N359 V363 C364 K365 M366 V372 F382 L410 V411 E412 L413 C420 E442 L448 N452 N453 V454 F455 N456 T457 N479 E486 F487 S488 R491 C498 S504 V508 G509 N510 K511 M512 F513 V514 K515 G516 A517 V521 V528 R529
V530 G531 T532 V535 P536 M537 K544 V548 I549 W552 C561 L562 A563 L564 A565 T566 R567 D568 E588 V596 M599 L600 D601 R604 K605 E606 V607 R615 I619 R620 V621 I622 E646 E647 V648 R651 F658 L663 R671 R672 A673 K686
L691 Q692 I697 T698 A699 M700 D703 N706 D707 L711 E715 I716 G717 I718 A719 S731 E732 M733 V734 L735 A736 D737 E749 I753 Y754 N755 N756 M757 F760 L764 I765 G770 E771 V772 C773 C774 I775 F776 L777 P784 E785 A786 L787 I788 P789 V790 Q791 L792
L793 W794 V795 V798 T799 P803 N810 D815 I816 M817 D818 R819 I829 L833 R836 Y837 I840 Y843 V844 A847 T848 V849 G850 A851 A852 A853 W854 W855 F856 A859 P863 G864 V865 T866 Q869 L870 F873 H874 GLN C876 T877 GLU D879 H882 F883
E884 G885 L886 D887 C888 E889 I890 F891 E892 A893 P894 E895 P896 M897 T898 M899 A900 L901 S902 V903 L904 V905 T906 I907 E908 N909 C910 S915 L916 S917 Q920 S921 R924 N925 P926 V929 L933 L934 I937 S940 M941 S942 L943 H944 F945 L946 I947 L948 L953 P954 F957
K958 L959 K960 A961 L962 D963 L964 T965 Q966 W967 L968 M969 V970 L971 K972 I973 S974 L975 P976 L980 K985 Y991 LEU GLU GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.14Å 94.39Å 135.11Å 90.00° 107.05° 90.00°	Depositor
Resolution (Å)	64.58 – 3.13 64.58 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.8 (64.58-3.13) 100.0 (64.58-3.13)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.201 , 0.259 0.205 , 0.261	Depositor DCC
R_{free} test set	2817 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	97.1	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 86.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15376	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, TG1, K, 128, MG, VN4

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	0.17	0/7704	0.39	0/10444
1	B	0.18	0/7735	0.39	2/10483 (0.0%)
All	All	0.17	0/15439	0.39	2/20927 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	703	ASP	N-CA-C	-5.14	108.76	114.62
1	B	865	VAL	N-CA-C	-5.11	106.60	112.98

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7569	0	7674	202	0
1	B	7599	0	7702	197	0
2	A	46	0	13	3	0
2	B	46	0	13	0	0
3	A	46	0	50	9	0
3	B	46	0	50	17	0
4	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	4	0	0	0	0
8	B	4	0	0	0	0
All	All	15376	0	15502	405	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 13.

All (405) 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:A:76:ALA:HB1	1:A:88:PHE:HD2	1.28	0.98
1:B:166:LEU:HD11	1:B:222:ILE:HG13	1.55	0.88
1:A:795:VAL:HA	1:A:799:THR:HB	1.62	0.80
1:B:104:VAL:HA	1:B:107:TRP:HD1	1.47	0.78
1:A:76:ALA:HB1	1:A:88:PHE:CD2	2.18	0.77
1:A:927:PRO:HB2	1:A:934:LEU:HD21	1.68	0.76
1:A:962:LEU:HB2	1:A:966:GLN:HB2	1.68	0.74
1:B:947:ILE:HG13	1:B:953:LEU:HB3	1.70	0.73
1:B:486:GLU:O	1:B:491:ARG:NH2	2.21	0.73
1:B:33:LEU:HD11	1:B:38:HIS:HD2	1.52	0.73
1:B:965:THR:OG1	1:B:966:GLN:OE1	2.05	0.73
1:B:357:THR:HG22	1:B:359:ASN:H	1.52	0.72
1:A:896:PRO:HA	1:A:899:MET:HE3	1.72	0.71
1:A:897:MET:SD	1:A:958:LYS:NZ	2.64	0.71
1:A:829:ILE:HD13	3:A:1001:TG1:H281	1.72	0.71
1:B:898:THR:HG22	1:B:958:LYS:HB3	1.72	0.71
1:B:119:LEU:HD23	1:B:236:ARG:HB3	1.74	0.69
1:B:648:VAL:HG13	1:B:651:ARG:HB2	1.72	0.69
1:A:260:LEU:HD12	3:A:1001:TG1:H261	1.73	0.69
1:B:799:THR:O	1:B:803:PRO:HD2	1.91	0.69
1:A:857:MET:HA	1:A:865:VAL:HA	1.76	0.68
1:B:884:GLU:O	1:B:886:LEU:N	2.26	0.68
1:B:906:THR:HG22	1:B:941:MET:HE1	1.75	0.68
1:A:869:GLN:NE2	1:A:882:HIS:HB3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HD11	1:B:38:HIS:CD2	2.30	0.67
3:B:2001:TG1:C22	3:B:2001:TG1:H312	2.24	0.67
1:A:396:LEU:HD23	1:A:399:ASP:HA	1.77	0.67
1:B:620:ARG:NH2	1:B:673:ALA:O	2.28	0.66
1:A:203:ASP:OD1	1:A:678:ARG:NH1	2.29	0.66
1:B:491:ARG:NH1	1:B:588:GLU:OE2	2.29	0.66
1:B:60:LEU:HD23	1:B:258:GLU:HA	1.77	0.66
1:A:866:THR:O	1:A:868:HIS:N	2.30	0.65
1:A:361:MET:HG3	1:A:599:MET:HG2	1.79	0.65
1:B:869:GLN:HG3	1:B:883:PHE:CD2	2.32	0.65
1:A:256:PHE:HD1	3:A:1001:TG1:HC6	1.62	0.65
1:B:967:TRP:HA	1:B:970:VAL:HG22	1.78	0.64
1:B:909:MET:HG3	1:B:937:ILE:HD12	1.78	0.64
1:A:829:ILE:HD13	3:A:1001:TG1:C28	2.28	0.64
1:A:155:VAL:HG12	1:A:216:ALA:HA	1.80	0.63
1:B:301:ALA:HA	1:B:789:PRO:HG3	1.80	0.63
1:B:413:LEU:HD22	1:B:452:MET:HE1	1.82	0.62
1:B:104:VAL:HA	1:B:107:TRP:CD1	2.33	0.62
1:A:646:GLU:OE2	1:A:651:ARG:NH1	2.32	0.62
1:A:650:ASP:O	1:A:672:ARG:NH1	2.33	0.62
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.80	0.61
1:A:876:CYS:SG	1:A:888:CYS:HB3	2.41	0.61
1:A:326:MET:HG3	1:A:331:ALA:HB3	1.83	0.61
1:B:719:ALA:HB3	1:B:734:VAL:HG12	1.82	0.61
1:A:8:SER:HB3	1:A:11:GLU:HG3	1.82	0.61
1:A:789:PRO:HA	1:A:792:LEU:HD12	1.82	0.60
1:A:252:LYS:NZ	1:A:826:GLU:O	2.34	0.60
1:A:333:VAL:HG22	1:A:733:MET:HE2	1.83	0.60
1:A:72:SER:HB3	1:A:91:PRO:HB3	1.83	0.60
1:B:785:GLU:HA	1:B:897:MET:HE2	1.83	0.60
1:A:495:SER:HB3	1:A:514:VAL:HG22	1.83	0.60
1:B:267:ILE:HG23	3:B:2001:TG1:H192	1.84	0.59
1:B:788:ILE:HG22	1:B:791:GLN:OE1	2.02	0.59
1:B:159:VAL:HG11	1:B:208:LEU:HB3	1.85	0.59
1:A:448:LEU:O	1:A:452:MET:HG2	2.03	0.59
1:B:529:ARG:HH22	1:B:568:ASP:CG	2.10	0.59
1:A:199:ALA:HB1	1:A:203:ASP:HB2	1.85	0.59
1:B:815:ASP:OD1	1:B:815:ASP:N	2.36	0.59
1:A:352:LYS:HE2	1:A:635:ILE:HG13	1.84	0.59
1:A:352:LYS:HE3	1:A:631:THR:HG22	1.84	0.58
1:A:79:GLU:O	1:A:83:GLU:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:VAL:HG11	1:A:339:VAL:HG22	1.86	0.58
1:B:863:PRO:HG3	1:B:886:LEU:HD22	1.86	0.58
1:A:346:SER:HB3	1:A:696:GLU:HB2	1.84	0.58
1:B:756:ASN:ND2	1:B:810:ASN:OD1	2.37	0.58
1:B:897:MET:SD	1:B:958:LYS:NZ	2.77	0.58
1:A:500:PRO:HD3	1:A:510:ASN:HB3	1.86	0.58
1:A:829:ILE:HA	1:A:833:LEU:HD12	1.84	0.58
1:A:950:VAL:O	1:A:954:PRO:HD2	2.04	0.57
1:B:363:VAL:HA	1:B:599:MET:HA	1.86	0.57
1:A:89:VAL:HG22	1:A:92:PHE:HB2	1.85	0.57
1:A:186:SER:O	2:A:1000:128:H5"	2.05	0.57
1:A:784:PRO:HB3	1:A:873:PHE:CZ	2.40	0.57
1:A:757:MET:HA	1:A:760:PHE:CE2	2.39	0.57
1:B:511:LYS:HD2	1:B:568:ASP:HA	1.86	0.57
1:A:981:ASP:O	1:A:985:LYS:N	2.34	0.57
1:A:26:PRO:HA	1:A:29:VAL:HG12	1.87	0.56
1:A:899:MET:HE2	1:A:966:GLN:OE1	2.04	0.56
1:B:840:ILE:O	1:B:844:VAL:HG23	2.06	0.56
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.87	0.56
1:A:907:ILE:HG13	1:A:977:VAL:HG11	1.88	0.56
1:B:944:HIS:O	1:B:947:ILE:HG22	2.06	0.56
1:A:511:LYS:HD2	1:A:568:ASP:HA	1.88	0.56
1:B:791:GLN:NE2	1:B:901:LEU:HB2	2.21	0.55
1:A:23:GLY:HA3	1:A:131:ARG:HA	1.88	0.55
1:B:155:VAL:HG22	1:B:217:GLY:H	1.71	0.55
1:A:851:ALA:HB1	1:A:899:MET:HB2	1.88	0.55
1:A:174:ARG:HB3	1:A:186:SER:HB3	1.89	0.55
1:B:966:GLN:OE1	1:B:966:GLN:N	2.40	0.55
1:A:806:ALA:HB1	1:A:933:LEU:HA	1.89	0.55
1:A:869:GLN:HE21	1:A:882:HIS:HB3	1.71	0.55
1:B:788:ILE:HG23	1:B:791:GLN:H	1.71	0.55
1:B:325:ARG:NH1	1:B:749:GLU:OE2	2.39	0.54
1:A:906:THR:HG22	1:A:941:MET:HE1	1.89	0.54
1:A:855:TRP:O	1:A:862:GLY:HA3	2.06	0.54
1:B:83:GLU:HG2	1:B:84:THR:O	2.08	0.54
1:B:266:LEU:HD13	3:B:2001:TG1:H191	1.89	0.54
1:B:342:LEU:HD23	1:B:716:ILE:HD13	1.90	0.54
1:B:855:TRP:HA	1:B:859:ALA:HB2	1.90	0.54
1:B:620:ARG:HH12	1:B:671:ARG:HA	1.73	0.54
1:A:868:HIS:O	1:A:871:THR:OG1	2.24	0.53
1:B:606:GLU:OE1	1:B:606:GLU:N	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:933:LEU:O	1:B:937:ILE:HG12	2.08	0.53
1:A:650:ASP:HB3	1:A:672:ARG:HH12	1.73	0.53
1:A:119:LEU:HD23	1:A:236:ARG:HB3	1.90	0.53
1:A:353:THR:HA	1:A:357:THR:OG1	2.08	0.53
1:A:662:PRO:HD3	1:B:198:ARG:HH12	1.72	0.53
1:B:887:ASP:O	1:B:890:ILE:HG22	2.08	0.53
1:A:739:ASN:O	1:A:742:THR:HG22	2.09	0.53
1:B:248:PRO:HD2	1:B:341:THR:HG22	1.90	0.52
1:A:185:VAL:HG21	2:A:1000:128:C8	2.39	0.52
1:B:35:LYS:HD3	1:B:36:TYR:CZ	2.44	0.52
1:B:899:MET:O	1:B:903:VAL:HG22	2.09	0.52
1:B:909:MET:SD	1:B:941:MET:HG2	2.49	0.52
1:B:413:LEU:HG	1:B:564:LEU:HD12	1.91	0.52
1:B:266:LEU:HD22	3:B:2001:TG1:H191	1.90	0.52
1:B:488:SER:HB3	1:B:491:ARG:HG2	1.92	0.52
1:B:962:LEU:HB2	1:B:966:GLN:OE1	2.10	0.52
1:A:340:GLU:OE1	1:A:822:ARG:NH2	2.43	0.52
1:A:614:CYS:HB3	1:A:619:ILE:HB	1.92	0.52
1:B:351:ASP:HB3	1:B:355:THR:OG1	2.09	0.52
1:A:899:MET:HB3	1:A:966:GLN:OE1	2.09	0.52
1:B:837:TYR:HA	1:B:840:ILE:HG22	1.92	0.52
1:A:650:ASP:CB	1:A:672:ARG:HH12	2.23	0.52
1:A:770:GLY:HA3	1:A:844:VAL:HG13	1.91	0.52
1:B:256:PHE:HE1	3:B:2001:TG1:H231	1.75	0.52
3:B:2001:TG1:O11	3:B:2001:TG1:H302	2.09	0.52
1:B:848:THR:HA	1:B:903:VAL:HG21	1.91	0.51
1:A:529:ARG:NH2	1:A:568:ASP:OD1	2.43	0.51
1:A:774:CYS:SG	1:A:787:LEU:HD23	2.51	0.51
1:B:174:ARG:HB3	1:B:186:SER:HB3	1.91	0.51
1:A:512:MET:HB2	1:A:567:ARG:HB3	1.93	0.51
1:A:836:ARG:HH12	1:A:919:ASN:H	1.59	0.51
1:A:78:PHE:HD2	1:A:293:ILE:HD11	1.76	0.51
1:B:330:ASN:HB3	1:B:737:ASP:H	1.76	0.51
1:B:363:VAL:HG21	1:B:448:LEU:HD22	1.92	0.51
1:B:959:LEU:HD12	1:B:960:LYS:H	1.75	0.51
3:B:2001:TG1:H233	3:B:2001:TG1:C5	2.40	0.51
1:B:515:LYS:HD2	1:B:562:LEU:HD13	1.92	0.51
1:B:549:ILE:HD11	1:B:596:VAL:HG21	1.92	0.51
1:B:13:LEU:HD23	1:B:222:ILE:HD11	1.93	0.50
1:B:528:VAL:HG23	1:B:537:MET:HB2	1.92	0.50
1:B:119:LEU:CD2	1:B:236:ARG:HB3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:GLU:HG3	1:B:897:MET:HE2	1.92	0.50
1:A:9:THR:HG21	1:A:191:THR:HG22	1.93	0.50
1:A:82:GLU:OE2	1:A:85:ILE:HD13	2.11	0.50
1:A:880:HIS:N	1:A:881:PRO:HD2	2.27	0.50
1:B:948:LEU:HB3	1:B:960:LYS:HD3	1.93	0.50
1:A:73:PHE:HE1	1:A:92:PHE:HE1	1.58	0.50
1:B:646:GLU:OE2	1:B:651:ARG:NH1	2.45	0.50
1:B:50:TRP:O	1:B:54:ILE:HG12	2.12	0.50
1:B:71:ILE:HG12	1:B:296:PHE:HD2	1.76	0.50
1:A:247:THR:HG22	1:A:249:LEU:H	1.77	0.50
1:B:944:HIS:O	1:B:948:LEU:HD12	2.12	0.50
1:A:785:GLU:HB2	1:A:852:ALA:HB1	1.93	0.49
1:A:414:ALA:HB3	1:A:454:VAL:HG21	1.94	0.49
1:A:498:CYS:O	1:A:510:ASN:HB2	2.12	0.49
1:B:1:MET:HG2	1:B:4:ALA:HB2	1.92	0.49
1:B:260:LEU:HD23	3:B:2001:TG1:C22	2.42	0.49
1:A:97:ILE:HG13	1:A:797:LEU:HD11	1.94	0.49
1:B:49:LEU:HA	1:B:52:LEU:HD12	1.93	0.49
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.93	0.49
1:A:663:LEU:HD21	1:B:663:LEU:HD13	1.95	0.49
1:A:974:SER:O	1:A:977:VAL:HG12	2.13	0.49
1:B:246:LYS:HB3	1:B:250:GLN:HG2	1.94	0.49
1:A:964:LEU:O	1:A:968:LEU:HG	2.12	0.49
1:B:866:THR:HG23	1:B:884:GLU:HG3	1.93	0.49
1:A:855:TRP:HB2	1:A:899:MET:HE1	1.94	0.49
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.94	0.49
1:B:166:LEU:HG	1:B:221:GLY:HA2	1.95	0.49
1:B:319:LEU:HB3	1:B:336:LEU:HD12	1.95	0.49
1:B:700:MET:HG3	1:B:711:LEU:HD12	1.95	0.49
1:B:917:SER:HB3	1:B:920:GLN:HB2	1.95	0.49
1:B:155:VAL:HG22	1:B:216:ALA:HA	1.95	0.49
1:B:165:ILE:HG22	1:B:191:THR:HG22	1.94	0.49
1:B:606:GLU:H	1:B:606:GLU:CD	2.21	0.49
3:B:2001:TG1:H233	3:B:2001:TG1:C4	2.43	0.49
1:B:753:ILE:O	1:B:757:MET:N	2.38	0.48
1:A:77:TRP:HA	1:A:77:TRP:CE3	2.48	0.48
1:A:255:GLU:O	1:A:259:GLN:HG2	2.13	0.48
1:A:764:LEU:O	1:A:768:ASN:ND2	2.40	0.48
1:B:757:MET:HA	1:B:760:PHE:CD2	2.48	0.48
1:B:887:ASP:OD1	1:B:888:CYS:N	2.46	0.48
1:B:357:THR:HG21	1:B:601:ASP:CG	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:LEU:H	1:A:814:LEU:HD23	1.78	0.48
1:A:187:VAL:HG12	1:A:189:LYS:HD3	1.95	0.48
1:A:311:LEU:HD23	1:A:764:LEU:HD12	1.94	0.48
1:A:648:VAL:HG13	1:A:651:ARG:HB2	1.96	0.48
1:B:454:VAL:HG23	1:B:455:PHE:CD1	2.48	0.48
1:B:788:ILE:O	1:B:791:GLN:HG2	2.13	0.48
1:B:795:VAL:HG21	1:B:901:LEU:HD11	1.95	0.48
1:A:944:HIS:O	1:A:948:LEU:HG	2.13	0.48
1:A:260:LEU:CD1	3:A:1001:TG1:H261	2.42	0.48
1:B:909:MET:SD	1:B:937:ILE:HG23	2.54	0.48
1:B:202:GLN:N	1:B:202:GLN:OE1	2.45	0.47
1:A:382:PHE:CD2	1:A:397:LYS:HB2	2.50	0.47
1:B:366:MET:HA	1:B:596:VAL:O	2.14	0.47
1:A:52:LEU:HD22	1:A:106:VAL:HG23	1.96	0.47
1:A:200:VAL:HG22	1:A:203:ASP:OD2	2.14	0.47
1:B:41:LEU:HD22	1:B:236:ARG:HD3	1.96	0.47
1:B:815:ASP:O	1:B:819:ARG:HG2	2.13	0.47
1:A:256:PHE:CD1	3:A:1001:TG1:HC6	2.46	0.47
1:A:453:ASN:ND2	1:A:457:THR:O	2.45	0.47
1:A:65:LEU:HD13	1:A:307:ILE:HD11	1.97	0.47
1:A:800:ASP:C	1:A:803:PRO:HD2	2.40	0.47
1:B:795:VAL:HG11	1:B:905:VAL:HG12	1.96	0.47
1:A:78:PHE:O	1:A:81:GLY:N	2.47	0.47
1:A:113:GLU:HG3	1:A:729:THR:HG23	1.97	0.47
3:A:1001:TG1:H311	3:A:1001:TG1:HC2	1.62	0.47
1:B:260:LEU:HD23	3:B:2001:TG1:H232	1.97	0.47
1:B:235:ILE:O	1:B:239:MET:HB2	2.15	0.47
1:B:969:MET:O	1:B:973:ILE:HG12	2.15	0.47
1:A:561:CYS:HA	1:A:597:VAL:O	2.15	0.46
1:A:606:GLU:HG3	1:A:739:ASN:OD1	2.14	0.46
1:B:44:GLU:OE1	1:B:114:ASN:ND2	2.48	0.46
1:B:412:GLU:OE2	1:B:566:THR:HG21	2.15	0.46
1:B:267:ILE:CG2	3:B:2001:TG1:H192	2.44	0.46
1:A:94:ILE:HG12	1:A:793:LEU:HD11	1.97	0.46
1:B:817:MET:HE3	1:B:817:MET:HA	1.97	0.46
1:A:41:LEU:HB3	1:A:236:ARG:CD	2.45	0.46
1:A:361:MET:HB3	1:A:444:ALA:HB2	1.98	0.46
1:A:572:LYS:HB2	1:A:575:GLU:HB2	1.96	0.46
1:B:976:PRO:O	1:B:980:LEU:N	2.39	0.46
1:A:357:THR:HA	1:A:603:PRO:HA	1.96	0.46
1:A:512:MET:HG3	1:A:570:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:TRP:HZ3	1:B:966:GLN:NE2	2.13	0.46
1:A:119:LEU:CD2	1:A:236:ARG:HB3	2.45	0.46
1:B:855:TRP:CD1	1:B:896:PRO:HB3	2.51	0.46
1:B:856:PHE:O	1:B:864:GLY:HA2	2.15	0.46
1:A:85:ILE:O	1:A:88:PHE:HD1	1.99	0.46
1:A:909:MET:SD	1:A:940:SER:OG	2.70	0.46
1:A:950:VAL:C	1:A:954:PRO:HD2	2.41	0.46
1:A:65:LEU:HD23	1:A:98:LEU:HD21	1.97	0.46
1:B:256:PHE:CE1	3:B:2001:TG1:H231	2.51	0.46
1:B:732:GLU:OE2	1:B:732:GLU:N	2.49	0.46
1:B:777:LEU:HD11	1:B:849:VAL:HG11	1.97	0.46
1:B:947:ILE:HD11	1:B:957:PHE:CD2	2.51	0.46
1:A:349:CYS:N	1:A:699:ALA:O	2.47	0.45
1:B:508:VAL:HB	1:B:510:ASN:OD1	2.16	0.45
1:B:879:ASP:HB2	1:B:882:HIS:CE1	2.51	0.45
1:B:920:GLN:H	1:B:985:LYS:HE2	1.80	0.45
1:A:560:ARG:HD2	1:A:560:ARG:HA	1.82	0.45
1:A:116:ILE:HD11	1:A:240:ALA:HB2	1.98	0.45
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.98	0.45
1:B:382:PHE:CE1	1:B:410:LEU:HD11	2.51	0.45
1:A:802:LEU:HG	1:A:939:LEU:HD22	1.98	0.45
1:A:933:LEU:O	1:A:937:ILE:HG13	2.17	0.45
1:B:305:ALA:HB1	1:B:771:GLU:HB3	1.99	0.45
1:B:848:THR:HG22	1:B:903:VAL:HG23	1.97	0.45
1:B:844:VAL:HG22	1:B:907:ILE:HG21	1.99	0.45
1:A:391:PRO:HB3	1:A:450:GLU:HB3	1.99	0.45
1:A:903:VAL:HA	1:A:970:VAL:HG13	1.99	0.45
1:A:930:ASN:ND2	1:A:933:LEU:HB2	2.32	0.45
1:B:113:GLU:HB2	1:B:334:ARG:HH22	1.82	0.45
1:A:804:ALA:HA	1:A:807:LEU:HD23	1.98	0.45
1:B:777:LEU:HD11	1:B:849:VAL:HG21	1.98	0.45
1:A:90:GLU:N	1:A:91:PRO:HD2	2.32	0.45
1:B:247:THR:HG21	1:B:337:PRO:HB2	1.99	0.45
1:B:784:PRO:HG3	1:B:873:PHE:HB3	1.99	0.45
1:A:336:LEU:O	1:A:339:VAL:HG23	2.17	0.44
1:B:926:PRO:O	1:B:929:VAL:HG12	2.18	0.44
1:A:52:LEU:HD13	1:A:106:VAL:HG23	1.98	0.44
1:B:692:GLN:HE21	1:B:715:GLU:HG2	1.81	0.44
1:A:59:ASP:HB3	1:A:62:VAL:HG22	1.98	0.44
1:B:287:SER:HB2	1:B:290:ARG:HB3	1.99	0.44
1:A:951:ASP:O	1:A:955:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:882:HIS:HD2	1:B:883:PHE:HB2	1.82	0.44
1:B:898:THR:HG22	1:B:958:LYS:HD2	2.00	0.44
1:B:152:GLU:HB2	1:B:220:LEU:HD12	1.99	0.44
1:A:840:ILE:O	1:A:844:VAL:HG12	2.17	0.44
1:B:140:ILE:HG13	1:B:141:LYS:O	2.17	0.44
1:B:963:ASP:OD1	1:B:963:ASP:N	2.51	0.44
1:A:6:SER:HA	1:A:194:VAL:O	2.18	0.44
1:B:267:ILE:HD11	1:B:302:LEU:HD11	1.99	0.44
1:B:784:PRO:HG3	1:B:873:PHE:CD1	2.53	0.44
1:B:905:VAL:HG21	1:B:944:HIS:CE1	2.53	0.44
1:B:733:MET:HE3	1:B:733:MET:HB2	1.75	0.44
1:A:559:LEU:HD22	1:A:600:LEU:HB2	2.00	0.43
1:A:103:ILE:HD13	1:A:103:ILE:HA	1.93	0.43
1:A:403:ARG:HB2	1:A:406:GLN:HG2	1.99	0.43
1:B:706:ASN:OD1	1:B:706:ASN:N	2.50	0.43
1:B:890:ILE:HA	1:B:893:ALA:HB2	2.00	0.43
1:A:342:LEU:HD13	1:A:716:ILE:HG21	2.00	0.43
1:A:944:HIS:O	1:A:947:ILE:HG12	2.18	0.43
1:B:329:LYS:HA	1:B:329:LYS:HD2	1.87	0.43
1:B:442:GLU:HG2	1:B:515:LYS:HZ1	1.83	0.43
1:A:264:ILE:HD11	1:A:306:ALA:HB1	2.00	0.43
1:A:905:VAL:O	1:A:909:MET:HG2	2.18	0.43
1:A:371:LYS:HD3	1:A:371:LYS:HA	1.80	0.43
1:A:909:MET:HG3	1:A:941:MET:HE2	1.99	0.43
1:A:256:PHE:CZ	1:A:765:ILE:HD12	2.54	0.43
1:A:865:VAL:HG12	1:A:866:THR:H	1.84	0.43
1:B:22:THR:HG22	1:B:23:GLY:O	2.17	0.43
1:A:85:ILE:O	1:A:88:PHE:CD1	2.72	0.43
1:A:97:ILE:HD13	1:A:97:ILE:HA	1.87	0.43
1:A:962:LEU:HB2	1:A:966:GLN:CB	2.43	0.43
1:B:975:LEU:N	1:B:976:PRO:HD2	2.34	0.43
1:A:678:ARG:HG3	6:A:1005:CL:CL	2.56	0.43
1:B:260:LEU:HD23	3:B:2001:TG1:C23	2.49	0.43
1:A:958:LYS:HA	1:A:958:LYS:HD3	1.81	0.42
1:B:719:ALA:HB2	1:B:731:SER:OG	2.19	0.42
3:B:2001:TG1:H302	3:B:2001:TG1:HO11	1.83	0.42
1:A:404:SER:HB3	1:A:410:LEU:HD23	2.00	0.42
1:A:868:HIS:CD2	1:A:868:HIS:H	2.36	0.42
1:A:103:ILE:HA	1:A:106:VAL:HG12	2.02	0.42
1:A:171:THR:OG1	1:A:486:GLU:OE1	2.35	0.42
1:B:99:ILE:HD13	1:B:99:ILE:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:909:MET:HE1	1:B:940:SER:HB3	2.01	0.42
1:A:77:TRP:HA	1:A:77:TRP:HE3	1.85	0.42
1:A:260:LEU:HD21	3:A:1001:TG1:H232	2.01	0.42
1:B:60:LEU:CD2	1:B:258:GLU:HA	2.46	0.42
1:A:41:LEU:HD13	1:A:236:ARG:HD2	2.00	0.42
1:A:604:ARG:HB2	1:A:607:VAL:HG23	2.01	0.42
1:A:943:LEU:O	1:A:947:ILE:HG23	2.20	0.42
1:B:498:CYS:O	1:B:510:ASN:HB3	2.19	0.42
1:A:236:ARG:HG3	1:A:237:ASP:N	2.33	0.42
1:A:840:ILE:HD13	1:A:980:LEU:HD23	2.02	0.42
1:B:604:ARG:HB2	1:B:607:VAL:HG23	2.01	0.42
1:B:829:ILE:HD12	1:B:833:LEU:HB3	2.02	0.42
1:B:895:GLU:HG3	1:B:959:LEU:HD23	2.01	0.42
1:B:953:LEU:N	1:B:954:PRO:HD2	2.35	0.42
1:A:25:THR:N	1:A:28:GLN:OE1	2.51	0.42
1:A:904:LEU:HA	1:A:907:ILE:HG22	2.02	0.42
1:B:308:PRO:O	1:B:311:LEU:HB3	2.20	0.42
1:B:791:GLN:O	1:B:795:VAL:HB	2.19	0.42
1:B:847:ALA:HB1	1:B:973:ILE:HG23	2.02	0.42
1:B:876:CYS:HB3	1:B:888:CYS:SG	2.59	0.42
1:A:363:VAL:HG11	1:A:448:LEU:HD22	2.02	0.42
1:B:332:ILE:HD13	1:B:736:ALA:HB2	2.01	0.42
1:B:345:THR:HA	1:B:697:ILE:HG22	2.01	0.42
1:A:962:LEU:O	1:A:966:GLN:N	2.34	0.42
1:A:975:LEU:HB3	1:A:976:PRO:HD3	2.00	0.42
1:B:870:LEU:HD12	1:B:891:PHE:CZ	2.55	0.42
1:A:247:THR:HB	1:A:250:GLN:HG2	2.02	0.42
1:A:369:ILE:H	1:A:369:ILE:HG12	1.71	0.42
1:A:715:GLU:C	1:A:716:ILE:HG13	2.45	0.42
1:A:737:ASP:C	1:A:739:ASN:H	2.28	0.42
1:B:85:ILE:HD12	1:B:85:ILE:H	1.85	0.42
1:A:116:ILE:HD13	1:A:236:ARG:HH21	1.85	0.41
1:A:963:ASP:OD1	1:A:963:ASP:N	2.52	0.41
1:B:200:VAL:O	1:B:204:LYS:HG3	2.20	0.41
1:B:622:ILE:HD12	1:B:691:LEU:HD11	2.02	0.41
1:B:869:GLN:H	1:B:869:GLN:HG2	1.42	0.41
1:B:366:MET:HE3	1:B:366:MET:HB2	1.88	0.41
1:A:625:THR:O	1:A:677:ALA:HA	2.20	0.41
1:A:985:LYS:O	1:A:989:ARG:HG2	2.21	0.41
1:B:787:LEU:HD23	1:B:791:GLN:NE2	2.36	0.41
1:B:855:TRP:HZ3	1:B:966:GLN:HE21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLY:HA3	1:A:130:TYR:O	2.20	0.41
1:A:412:GLU:OE2	1:A:566:THR:HG21	2.20	0.41
1:B:698:THR:O	1:B:715:GLU:HB2	2.20	0.41
1:B:895:GLU:CG	1:B:959:LEU:HD23	2.50	0.41
1:A:65:LEU:HG	1:A:98:LEU:HD11	2.03	0.41
1:A:383:SER:O	1:A:396:LEU:N	2.42	0.41
1:A:452:MET:O	1:A:454:VAL:HG23	2.21	0.41
1:A:921:SER:HB2	1:A:989:ARG:NH1	2.35	0.41
1:B:177:GLN:OE1	1:B:189:LYS:NZ	2.25	0.41
1:A:90:GLU:HB2	1:A:790:VAL:HG22	2.03	0.41
1:A:606:GLU:H	1:A:606:GLU:CD	2.29	0.41
1:B:266:LEU:O	1:B:269:VAL:HG12	2.20	0.41
1:B:770:GLY:O	1:B:773:VAL:HG22	2.21	0.41
1:A:485:LEU:HD22	1:A:584:PHE:CE1	2.56	0.41
1:A:765:ILE:O	1:A:769:VAL:HG13	2.20	0.41
1:B:311:LEU:HD13	1:B:764:LEU:HD12	2.02	0.41
1:B:517:ALA:O	1:B:521:VAL:HG13	2.21	0.41
1:B:833:LEU:HA	1:B:836:ARG:HB3	2.02	0.41
1:A:247:THR:HB	1:A:250:GLN:CG	2.51	0.41
1:A:831:GLY:O	1:A:834:PHE:HB3	2.20	0.41
1:B:302:LEU:HD21	1:B:772:VAL:HG13	2.03	0.41
1:B:658:PHE:HE1	1:B:686:LYS:HE3	1.85	0.41
1:B:757:MET:HA	1:B:760:PHE:CE2	2.55	0.41
1:B:947:ILE:HA	1:B:953:LEU:HD13	2.02	0.41
3:B:2001:TG1:H312	3:B:2001:TG1:C23	2.51	0.41
1:A:844:VAL:HG23	1:A:907:ILE:HG21	2.03	0.41
1:A:855:TRP:O	1:A:859:ALA:HB3	2.21	0.41
1:B:253:LEU:HA	1:B:256:PHE:HB3	2.02	0.41
1:B:365:LYS:HB3	1:B:552:TRP:CH2	2.56	0.41
1:A:18:VAL:HG11	1:A:24:LEU:HD12	2.03	0.40
1:A:828:LEU:HD13	3:A:1001:TG1:H291	2.02	0.40
1:B:266:LEU:HD22	3:B:2001:TG1:C19	2.52	0.40
1:A:581:SER:HA	1:A:584:PHE:CE2	2.56	0.40
1:A:599:MET:HE3	1:A:599:MET:HB2	1.86	0.40
1:A:622:ILE:HD12	1:A:691:LEU:HD11	2.03	0.40
1:B:372:VAL:HG11	1:B:535:VAL:HG21	2.02	0.40
1:B:707:ASP:HB3	1:B:711:LEU:HD13	2.03	0.40
1:B:921:SER:HB3	1:B:924:ARG:HG2	2.02	0.40
1:A:441:THR:OG1	2:A:1000:128:H1'	2.22	0.40
1:A:739:ASN:HD21	1:A:741:SER:HB2	1.87	0.40
1:A:894:PRO:HA	1:A:958:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:PRO:HD2	1:B:785:GLU:OE1	2.21	0.40
1:B:847:ALA:HB1	1:B:973:ILE:CG2	2.51	0.40
1:A:518:PRO:HA	1:A:563:ALA:HB2	2.02	0.40
1:A:784:PRO:HB3	1:A:873:PHE:CE1	2.57	0.40
1:A:799:THR:HG21	1:A:905:VAL:HG22	2.02	0.40
1:A:853:ALA:HB1	1:A:857:MET:SD	2.61	0.40
1:B:65:LEU:HB2	1:B:307:ILE:HD13	2.04	0.40
1:B:108:GLN:HA	1:B:336:LEU:HB2	2.02	0.40
1:B:168:ILE:HD13	1:B:173:LEU:HB3	2.03	0.40
1:B:798:VAL:HG11	1:B:943:LEU:HD23	2.03	0.40
1:B:757:MET:HG2	1:B:760:PHE:HE2	1.87	0.40
3:B:2001:TG1:H312	3:B:2001:TG1:C24	2.51	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	976/994 (98%)	930 (95%)	43 (4%)	3 (0%)	36	64
1	B	977/994 (98%)	919 (94%)	55 (6%)	3 (0%)	36	64
All	All	1953/1988 (98%)	1849 (95%)	98 (5%)	6 (0%)	36	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	867	TYR
1	B	885	GLY
1	A	865	VAL
1	B	278	HIS
1	B	891	PHE
1	A	274	ILE

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	827/840 (98%)	786 (95%)	41 (5%)	22 49
1	B	832/840 (99%)	791 (95%)	41 (5%)	22 49
All	All	1659/1680 (99%)	1577 (95%)	82 (5%)	22 49

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	64	ILE
1	A	74	VAL
1	A	77	TRP
1	A	103	ILE
1	A	116	ILE
1	A	121	GLU
1	A	149	ASP
1	A	185	VAL
1	A	225	THR
1	A	228	VAL
1	A	297	LYS
1	A	304	VAL
1	A	309	GLU
1	A	341	THR
1	A	350	SER
1	A	368	ILE
1	A	399	ASP
1	A	446	THR
1	A	464	LYS
1	A	478	LEU
1	A	486	GLU
1	A	519	GLU
1	A	524	ARG
1	A	533	THR
1	A	554	THR
1	A	574	GLU

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Mol	Chain	Res	Type
1	A	599	MET
1	A	611	ILE
1	A	679	VAL
1	A	729	THR
1	A	775	ILE
1	A	807	LEU
1	A	833	LEU
1	A	865	VAL
1	A	867	TYR
1	A	886	LEU
1	A	898	THR
1	A	950	VAL
1	A	959	LEU
1	A	962	LEU
1	B	22	THR
1	B	75	LEU
1	B	98	LEU
1	B	99	ILE
1	B	106	VAL
1	B	116	ILE
1	B	136	SER
1	B	137	VAL
1	B	232	ILE
1	B	276	ILE
1	B	289	ILE
1	B	316	THR
1	B	347	VAL
1	B	363	VAL
1	B	457	THR
1	B	508	VAL
1	B	521	VAL
1	B	530	VAL
1	B	532	THR
1	B	535	VAL
1	B	544	LYS
1	B	596	VAL
1	B	615	ARG
1	B	619	ILE
1	B	663	LEU
1	B	718	ILE
1	B	765	ILE
1	B	787	LEU

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Mol	Chain	Res	Type
1	B	788	ILE
1	B	790	VAL
1	B	793	LEU
1	B	817	MET
1	B	869	GLN
1	B	879	ASP
1	B	890	ILE
1	B	902	SER
1	B	905	VAL
1	B	924	ARG
1	B	943	LEU
1	B	946	LEU
1	B	962	LEU

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	612	GLN
1	A	759	GLN
1	A	796	ASN
1	A	868	HIS
1	A	869	GLN
1	A	914	ASN
1	A	930	ASN
1	B	108	GLN
1	B	278	HIS
1	B	280	ASN
1	B	692	GLN
1	B	756	ASN
1	B	768	ASN
1	B	882	HIS
1	B	920	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	128	B	2000	5	37,50,50	2.91	17 (45%)	49,80,80	3.24	22 (44%)
4	VN4	A	1002	1,8,5	0,3,3	-	-	-		
3	TG1	A	1001	-	43,48,48	0.90	0	44,72,72	1.00	2 (4%)
2	128	A	1000	5	37,50,50	2.98	16 (43%)	49,80,80	3.04	20 (40%)
4	VN4	B	2002	1,8,5	0,3,3	-	-	-		
3	TG1	B	2001	-	43,48,48	0.88	2 (4%)	44,72,72	0.99	1 (2%)

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	128	B	2000	5	-	6/26/80/80	0/5/5/5
3	TG1	A	1001	-	-	10/33/99/99	0/3/3/3
3	TG1	B	2001	-	-	19/33/99/99	0/3/3/3
2	128	A	1000	5	-	2/26/80/80	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	128	O2'-C1F	9.77	1.54	1.41
2	B	2000	128	O2'-C1F	9.63	1.54	1.41
2	A	1000	128	O3'-C1F	8.70	1.53	1.41
2	B	2000	128	O3'-C1F	8.45	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	128	C5F-C6F	4.91	1.51	1.37
2	B	2000	128	C5F-C6F	4.76	1.51	1.37
2	A	1000	128	C5'-C4'	3.47	1.62	1.51
2	A	1000	128	PB-O2B	-3.38	1.39	1.55
2	B	2000	128	PB-O2B	-3.35	1.39	1.55
2	B	2000	128	C5'-C4'	3.29	1.61	1.51
2	A	1000	128	C4-N3	3.19	1.40	1.34
2	B	2000	128	C2'-C3'	3.16	1.60	1.53
2	A	1000	128	PG-O1G	3.03	1.60	1.50
2	B	2000	128	PG-O1G	3.02	1.60	1.50
2	B	2000	128	C4-N3	3.01	1.40	1.34
2	A	1000	128	C2'-C3'	3.00	1.59	1.53
2	B	2000	128	C3'-C4'	-2.82	1.45	1.52
2	A	1000	128	C3'-C4'	-2.79	1.45	1.52
2	B	2000	128	C6-N1	2.71	1.43	1.35
2	A	1000	128	C6-N1	2.70	1.43	1.35
2	A	1000	128	C5-N7	-2.59	1.34	1.39
2	B	2000	128	C5-N7	-2.52	1.34	1.39
2	A	1000	128	PB-O1B	-2.43	1.42	1.50
2	B	2000	128	PB-O1B	-2.41	1.42	1.50
2	A	1000	128	C2-N3	2.36	1.38	1.33
2	B	2000	128	PG-O3G	-2.35	1.45	1.54
2	A	1000	128	PG-O3G	-2.32	1.45	1.54
2	A	1000	128	C2-N1	2.30	1.38	1.33
2	B	2000	128	O2'-C2'	2.30	1.46	1.43
2	B	2000	128	PA-O1A	2.29	1.59	1.50
2	A	1000	128	PA-O1A	2.25	1.58	1.50
2	B	2000	128	C2-N1	2.23	1.38	1.33
3	B	2001	TG1	C1-C5	2.14	1.54	1.51
3	B	2001	TG1	C2-C3	2.14	1.57	1.53
2	B	2000	128	C2-N3	2.06	1.37	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2000	128	O3'-C1F-C6F	-9.68	97.22	110.47
2	A	1000	128	C5-C4-N3	-7.97	116.34	126.75
2	B	2000	128	C5-C4-N3	-7.44	117.04	126.75
2	A	1000	128	C4'-O4'-C1'	7.36	125.71	109.47
2	B	2000	128	C4'-O4'-C1'	7.09	125.11	109.47
2	A	1000	128	O3'-C1F-C6F	-6.72	101.27	110.47
2	A	1000	128	N3-C4-N9	6.20	137.30	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2000	128	N3-C4-N9	5.58	136.28	127.08
2	B	2000	128	PB-O3B-PG	-5.37	114.41	132.83
2	A	1000	128	C2-N3-C4	5.15	123.92	111.75
2	B	2000	128	C2-N3-C4	5.10	123.79	111.75
2	A	1000	128	O4'-C1'-C2'	-4.96	97.87	106.57
2	A	1000	128	O2'-C1F-C2F	-4.95	103.69	110.47
2	B	2000	128	O2'-C1F-C6F	4.95	117.24	110.47
2	B	2000	128	N3-C2-N1	-4.90	120.94	128.60
2	A	1000	128	O2'-C2'-C3'	4.82	111.28	103.58
2	B	2000	128	O2'-C2'-C3'	4.81	111.27	103.58
2	A	1000	128	N3-C2-N1	-4.77	121.15	128.60
2	A	1000	128	PB-O3B-PG	-4.48	117.45	132.83
2	B	2000	128	O4'-C1'-C2'	-4.43	98.79	106.57
2	B	2000	128	C5'-C4'-C3'	4.05	127.83	114.40
2	A	1000	128	PA-O3A-PB	3.75	145.69	132.83
2	B	2000	128	PA-O3A-PB	3.61	145.21	132.83
2	A	1000	128	O3G-PG-O3B	3.43	116.14	104.64
2	B	2000	128	O3G-PG-O3B	3.42	116.10	104.64
2	B	2000	128	C1'-N9-C8	3.38	134.76	127.14
2	B	2000	128	C2'-C1'-N9	3.34	119.16	113.53
3	A	1001	TG1	C10-C1-C5	-3.02	111.65	115.26
2	A	1000	128	O3'-C3'-C2'	3.01	108.39	103.58
2	A	1000	128	O4'-C4'-C3'	-2.82	98.83	104.87
2	A	1000	128	C2'-C3'-C4'	2.80	110.36	103.72
2	A	1000	128	C6-C5-C4	2.78	120.93	117.18
2	B	2000	128	C2'-C3'-C4'	2.76	110.28	103.72
2	B	2000	128	O3'-C3'-C2'	2.69	107.88	103.58
2	B	2000	128	O4'-C4'-C3'	-2.64	99.21	104.87
2	B	2000	128	O2'-C1F-C2F	-2.51	107.03	110.47
2	A	1000	128	C5'-C4'-C3'	2.38	122.30	114.40
2	B	2000	128	C6-C5-C4	2.35	120.35	117.18
3	B	2001	TG1	O7-C27-O8	-2.28	118.19	123.70
2	A	1000	128	C1'-N9-C8	2.26	132.25	127.14
2	B	2000	128	C4-N9-C1'	-2.15	121.47	126.59
2	B	2000	128	O2A-PA-O5'	2.14	117.67	107.75
2	A	1000	128	C4-N9-C8	-2.10	103.45	105.73
3	A	1001	TG1	C26-C4-C5	-2.02	124.77	129.82
2	A	1000	128	O2'-C1F-C6F	2.01	113.22	110.47

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	128	O4'-C4'-C5'-O5'
2	B	2000	128	C5'-O5'-PA-O1A
2	B	2000	128	C5'-O5'-PA-O2A
2	B	2000	128	C5'-O5'-PA-O3A
2	B	2000	128	O4'-C4'-C5'-O5'
3	A	1001	TG1	C9-C8-O7-C27
3	A	1001	TG1	C31-C10-O9-C32
3	A	1001	TG1	O10-C32-O9-C10
3	A	1001	TG1	C33-C32-O9-C10
3	B	2001	TG1	C31-C10-O9-C32
3	B	2001	TG1	C3-C2-O1-C13
3	B	2001	TG1	C14-C13-O1-C2
3	B	2001	TG1	C2-C3-O3-C21
3	B	2001	TG1	C22-C21-O3-C3
3	B	2001	TG1	O10-C32-O9-C10
3	B	2001	TG1	C33-C32-O9-C10
3	A	1001	TG1	O8-C27-O7-C8
3	B	2001	TG1	O2-C13-O1-C2
3	A	1001	TG1	C28-C27-O7-C8
3	B	2001	TG1	O4-C21-O3-C3
2	B	2000	128	C3'-C4'-C5'-O5'
3	A	1001	TG1	C15-C16-C17-C18
3	B	2001	TG1	C15-C16-C17-C18
3	B	2001	TG1	C14-C15-C16-C17
3	B	2001	TG1	C17-C18-C19-C20
3	B	2001	TG1	O7-C27-C28-C29
3	A	1001	TG1	C16-C17-C18-C19
2	A	1000	128	C5'-O5'-PA-O3A
3	B	2001	TG1	C16-C17-C18-C19
3	B	2001	TG1	C9-C8-O7-C27
3	A	1001	TG1	C9-C10-O9-C32
2	B	2000	128	PA-O3A-PB-O2B
3	B	2001	TG1	O8-C27-C28-C29
3	A	1001	TG1	C7-C8-O7-C27
3	B	2001	TG1	C7-C8-O7-C27
3	B	2001	TG1	C27-C28-C29-C30
3	B	2001	TG1	C1-C10-O9-C32

There are no ring outliers.

3 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	TG1	9	0

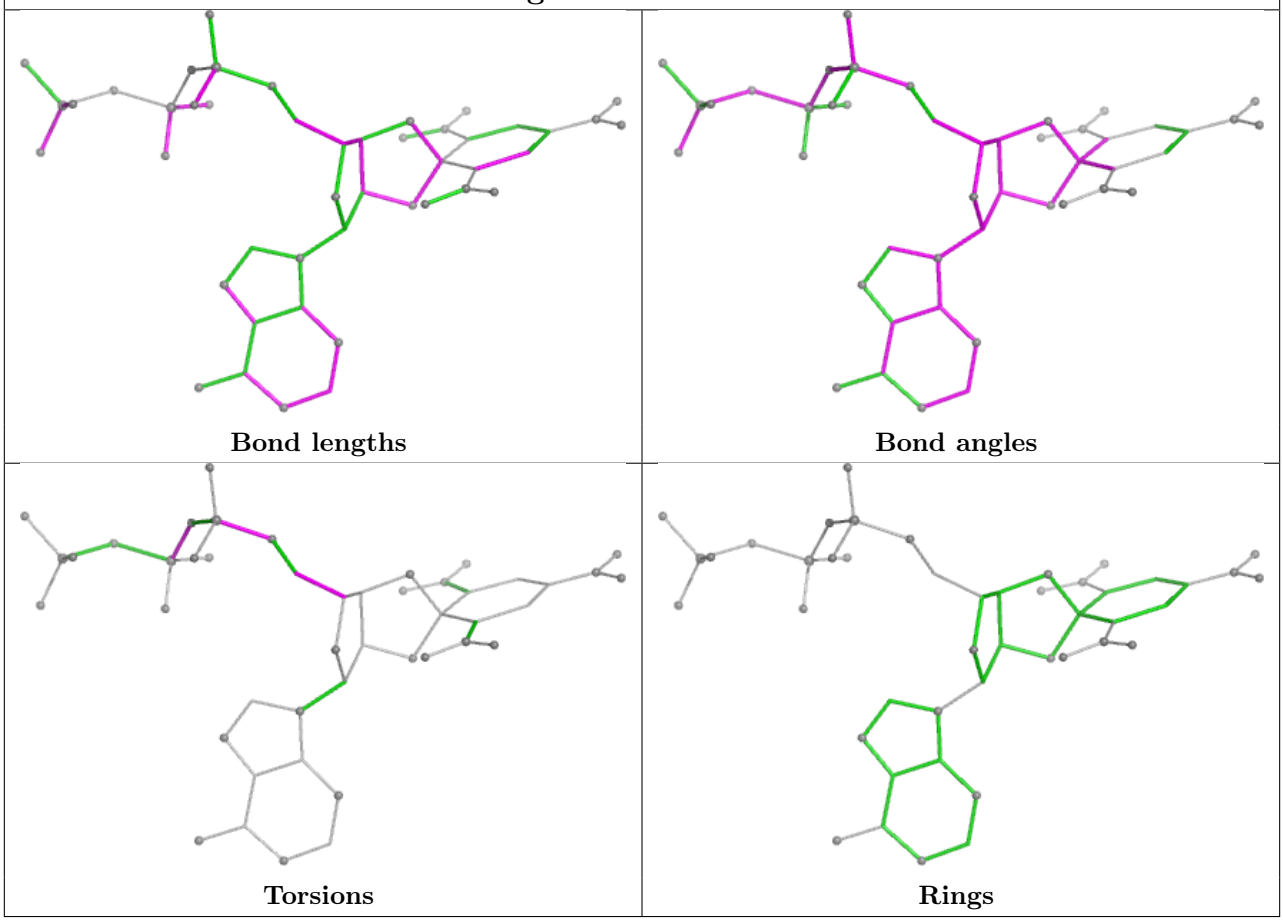
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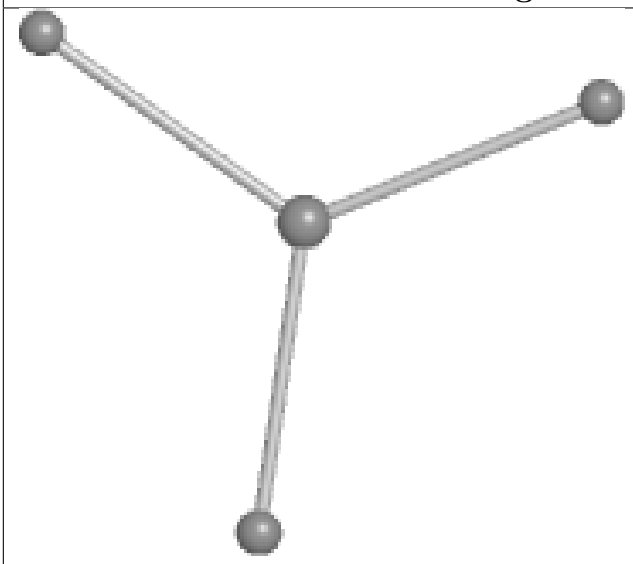
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	128	3	0
3	B	2001	TG1	17	0

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.

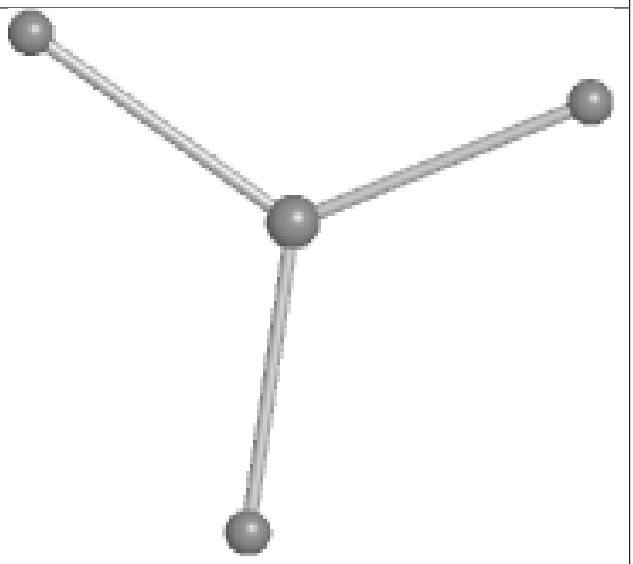
Ligand 128 B 2000



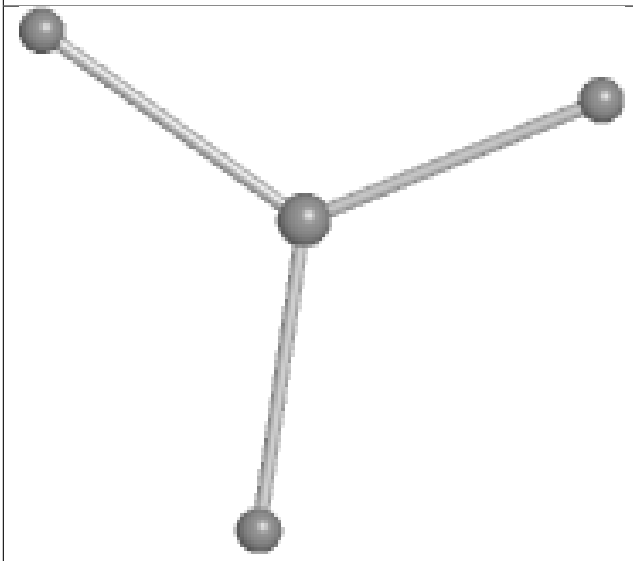
Ligand VN4 A 1002



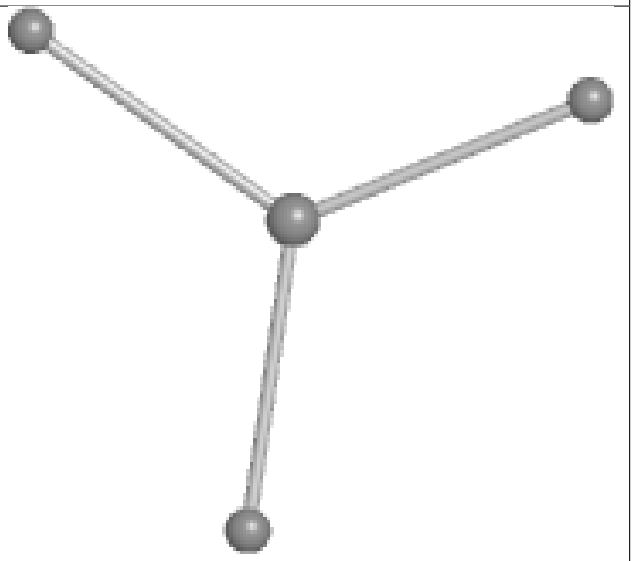
Bond lengths



Bond angles

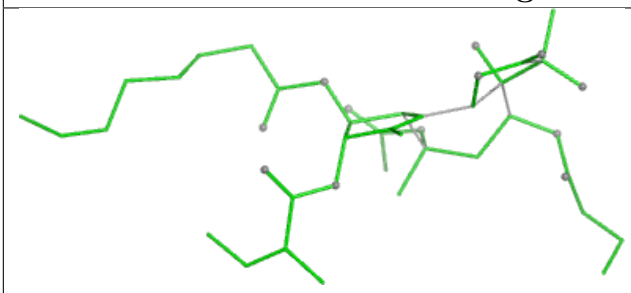


Torsions

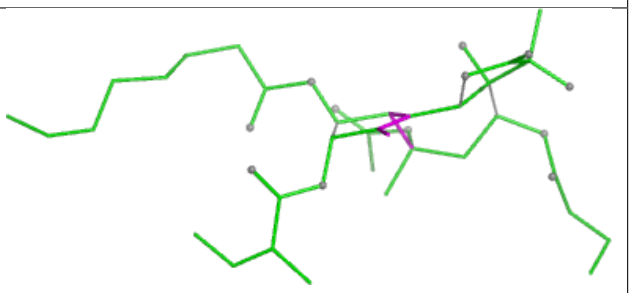


Rings

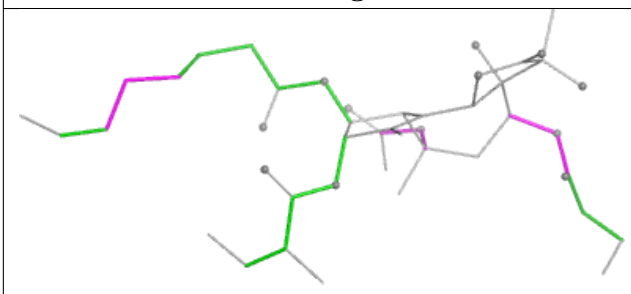
Ligand TG1 A 1001



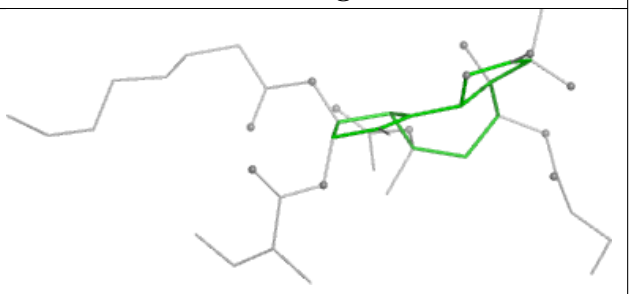
Bond lengths



Bond angles

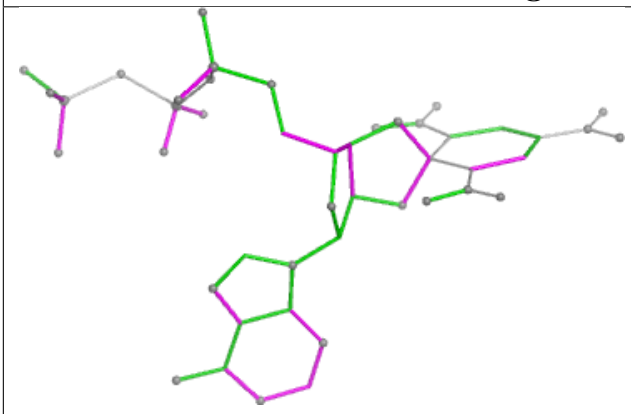


Torsions

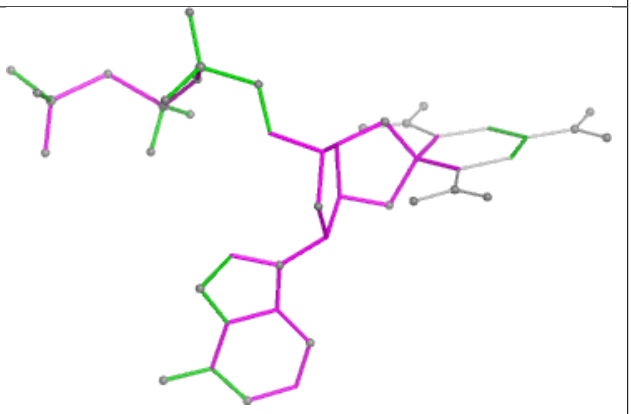


Rings

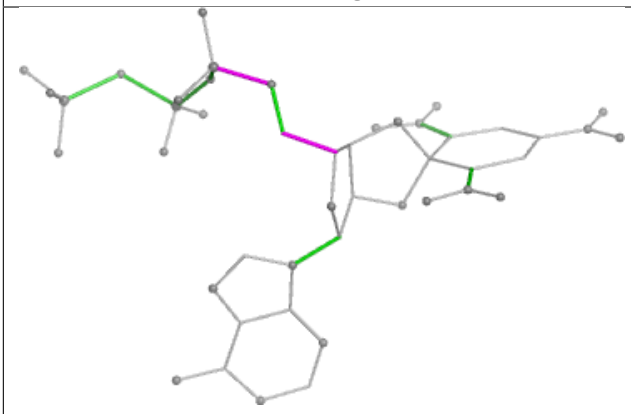
Ligand 128 A 1000



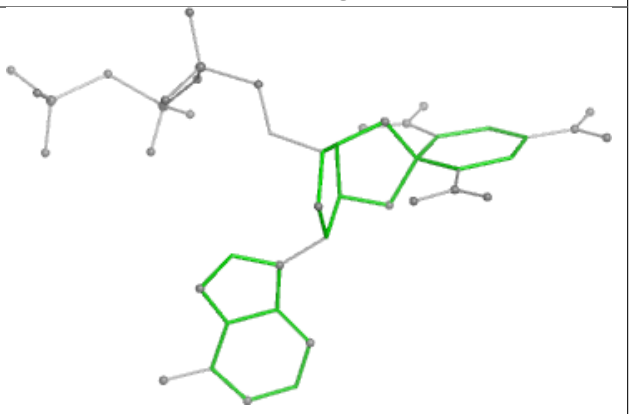
Bond lengths



Bond angles

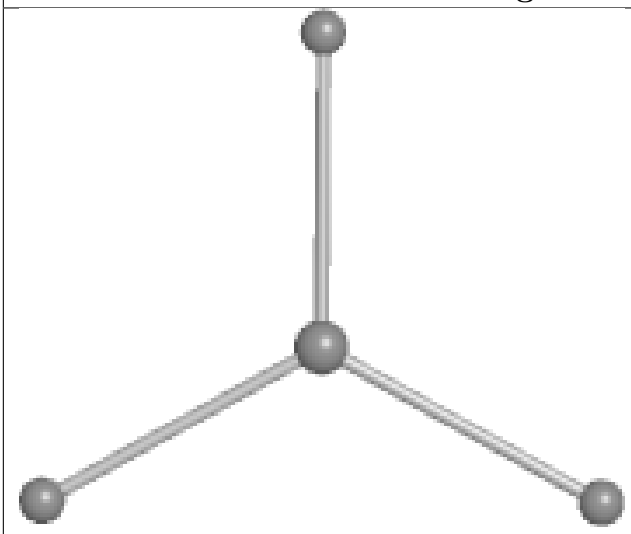


Torsions

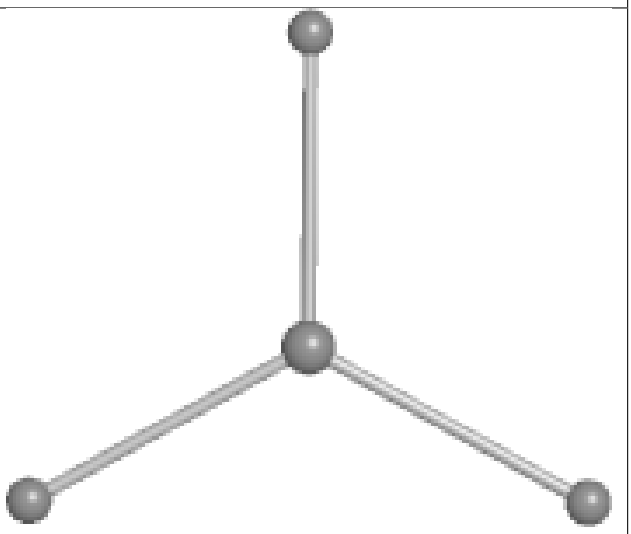


Rings

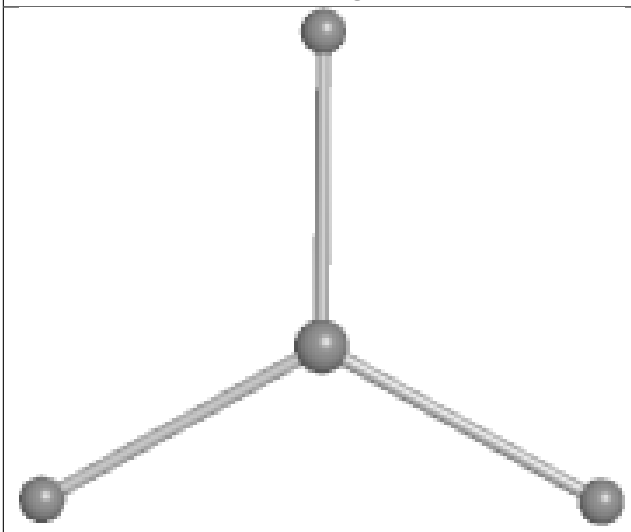
Ligand VN4 B 2002



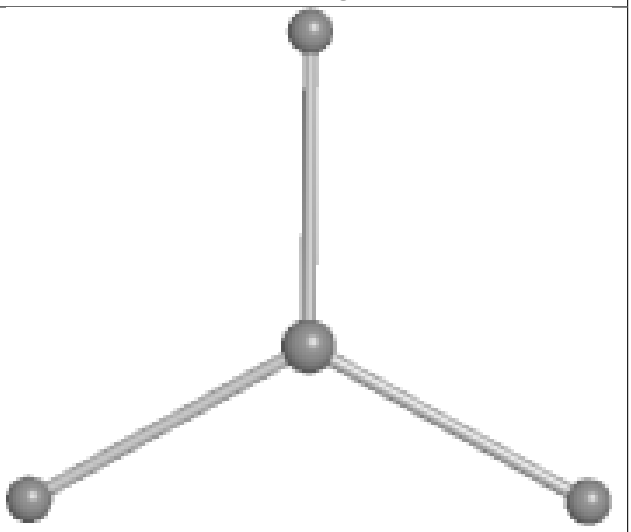
Bond lengths



Bond angles

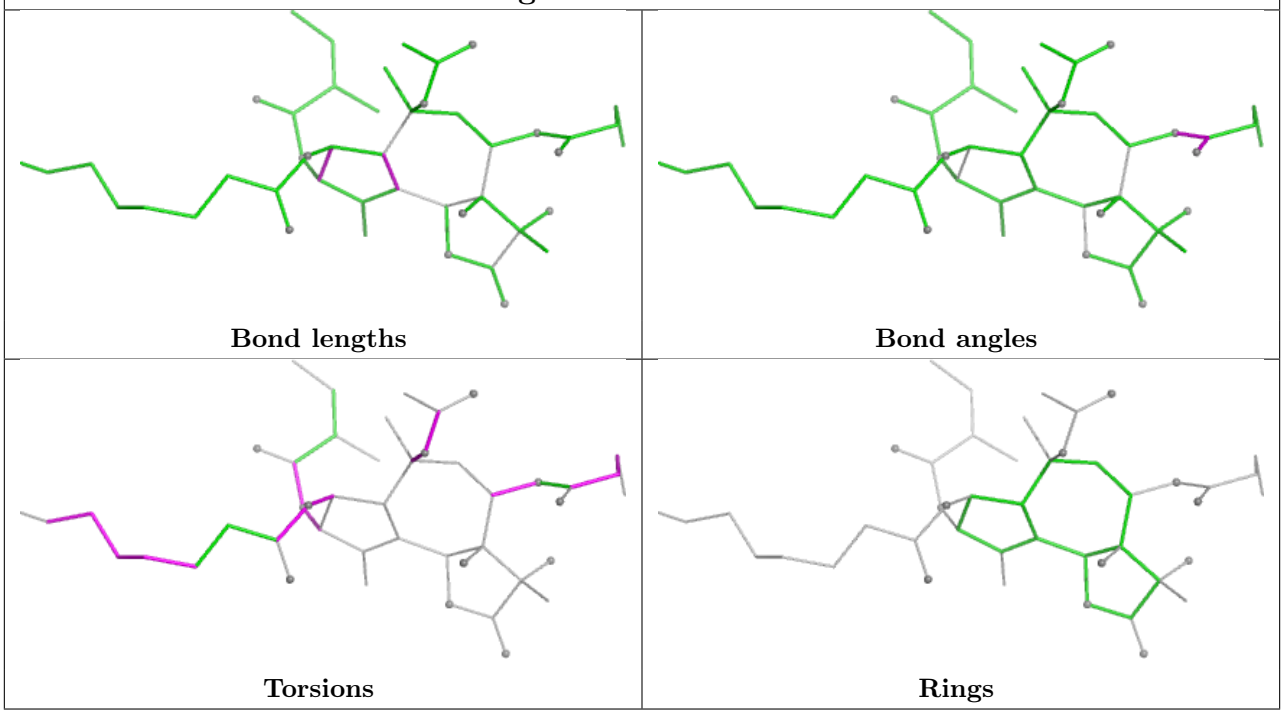


Torsions



Rings

Ligand TG1 B 2001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	982/994 (98%)	-0.02	21 (2%)	63	42	57, 100, 213, 290	0
1	B	985/994 (99%)	0.11	37 (3%)	44	24	60, 117, 220, 312	0
All	All	1967/1988 (98%)	0.05	58 (2%)	53	32	57, 110, 216, 312	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	971	LEU	4.4
1	B	852	ALA	3.9
1	A	968	LEU	3.4
1	B	865	VAL	3.4
1	A	786	ALA	3.4
1	B	791	GLN	3.3
1	B	754	TYR	3.3
1	B	504	SER	3.3
1	B	788	ILE	3.3
1	B	787	LEU	3.2
1	A	508	VAL	3.2
1	B	561	CYS	3.1
1	A	959	LEU	3.1
1	B	886	LEU	3.0
1	B	934	LEU	3.0
1	A	364	CYS	2.9
1	B	971	LEU	2.9
1	B	885	GLY	2.8
1	B	915	SER	2.8
1	B	775	ILE	2.7
1	B	786	ALA	2.7
1	A	785	GLU	2.7
1	B	884	GLU	2.6
1	A	242	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	851	ALA	2.5
1	B	853	ALA	2.5
1	A	113	GLU	2.4
1	A	44	GLU	2.4
1	A	974	SER	2.4
1	B	479	MET	2.4
1	B	785	GLU	2.4
1	B	61	LEU	2.3
1	B	925	MET	2.3
1	B	771	GLU	2.3
1	A	890	ILE	2.3
1	A	628	ASN	2.3
1	B	107	TRP	2.2
1	B	967	TRP	2.2
1	B	513	PHE	2.2
1	A	240	ALA	2.2
1	B	562	LEU	2.2
1	B	899	MET	2.2
1	B	945	PHE	2.2
1	B	906	THR	2.1
1	B	329	LYS	2.1
1	A	276	ILE	2.1
1	A	88	PHE	2.1
1	A	552	TRP	2.1
1	B	843	TYR	2.1
1	B	974	SER	2.1
1	A	273	LEU	2.1
1	A	241	ALA	2.1
1	B	548	VAL	2.1
1	A	864	GLY	2.1
1	A	561	CYS	2.0
1	B	420	CYS	2.0
1	B	498	CYS	2.0
1	B	910	CYS	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)

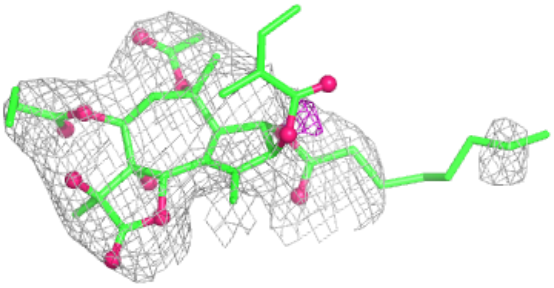
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

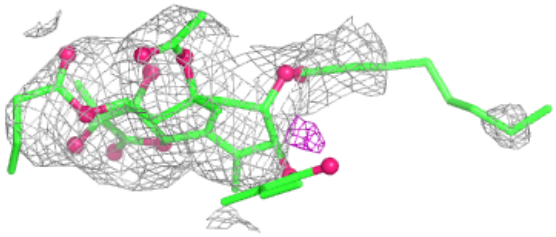
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	1004	1/1	0.62	0.31	296,296,296,296	0
3	TG1	B	2001	46/46	0.86	0.13	120,152,192,200	0
2	128	A	1000	46/46	0.90	0.15	90,124,244,292	0
3	TG1	A	1001	46/46	0.90	0.13	128,150,165,179	0
7	K	B	2006	1/1	0.90	0.10	109,109,109,109	0
2	128	B	2000	46/46	0.92	0.13	117,146,189,204	0
6	CL	A	1005	1/1	0.94	0.33	80,80,80,80	0
6	CL	B	2005	1/1	0.95	0.09	94,94,94,94	0
4	VN4	A	1002	4/4	0.95	0.15	92,100,102,117	0
5	MG	B	2004	1/1	0.97	0.05	122,122,122,122	0
4	VN4	B	2002	4/4	0.98	0.08	96,99,121,122	0
5	MG	A	1003	1/1	0.99	0.10	98,98,98,98	0
7	K	A	1006	1/1	0.99	0.04	103,103,103,103	0
5	MG	B	2003	1/1	0.99	0.04	93,93,93,93	0

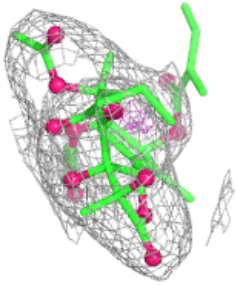
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TG1 B 2001:

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

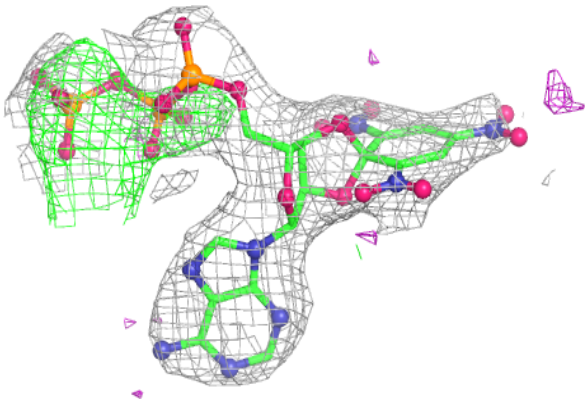


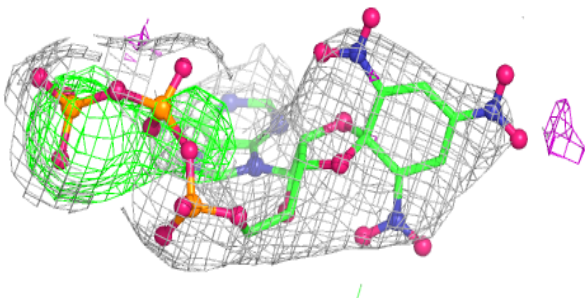


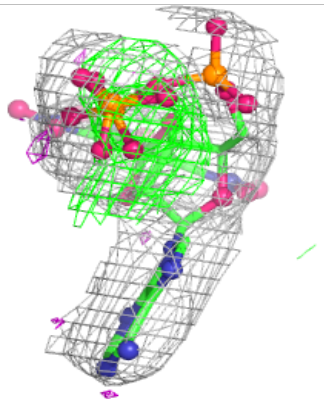


Electron density around 128 A 1000:

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

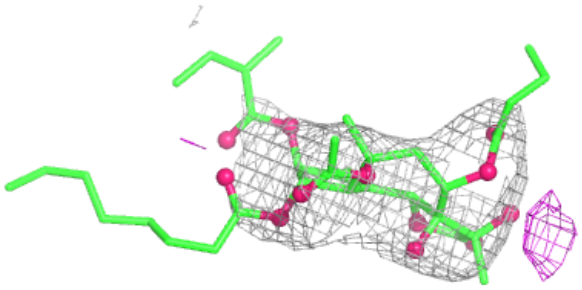


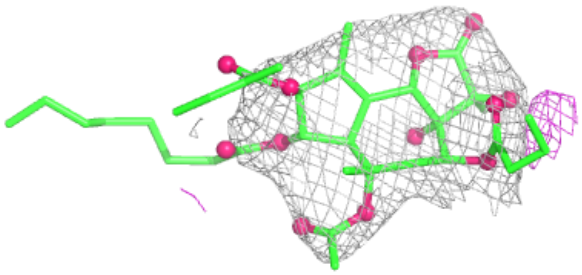


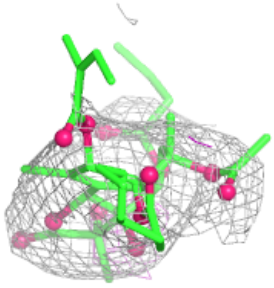


Electron density around TG1 A 1001:

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

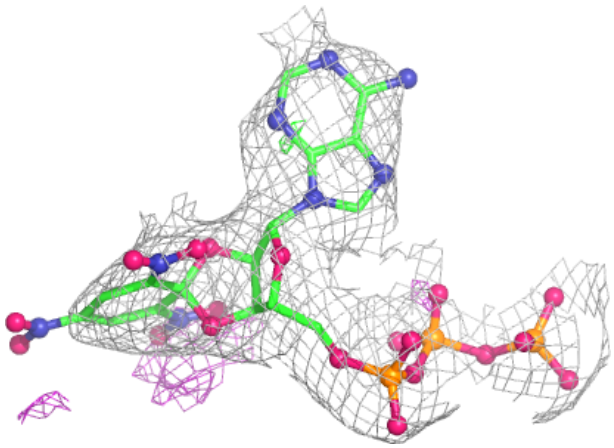


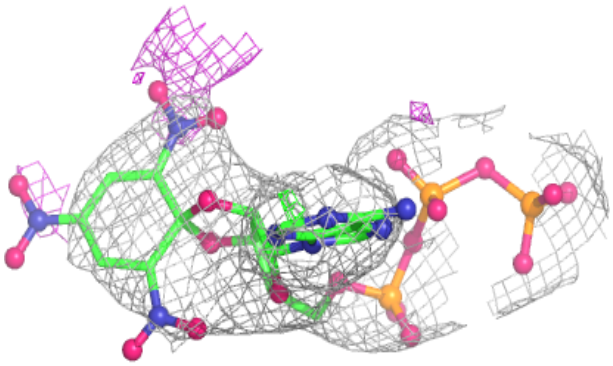


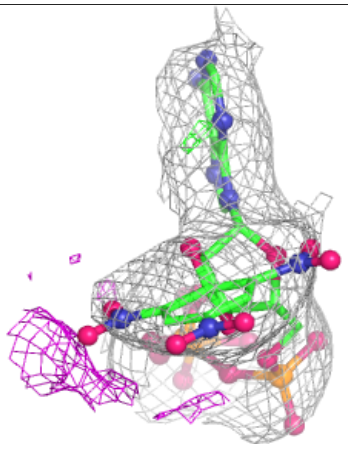


Electron density around 128 B 2000:

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

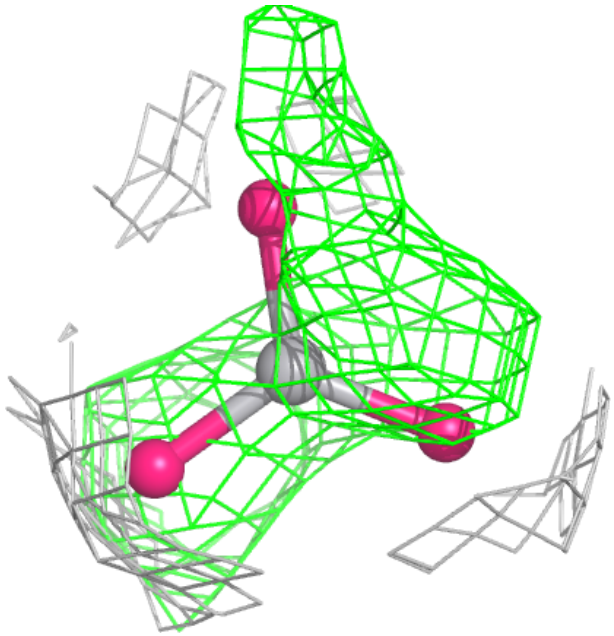


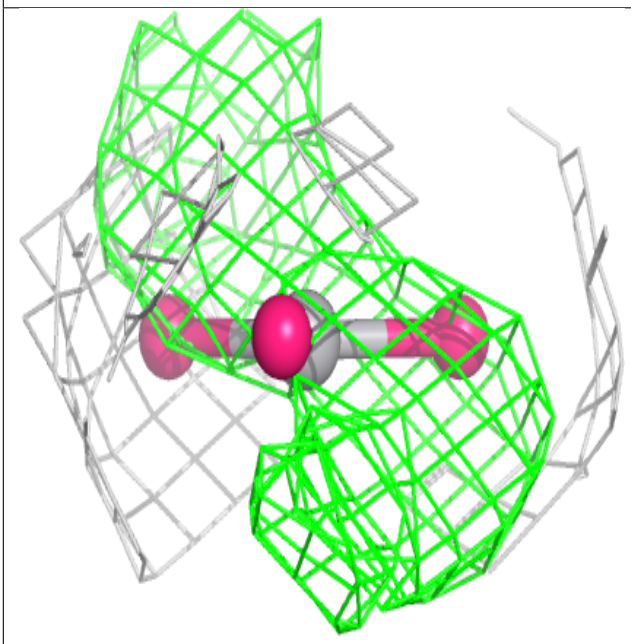


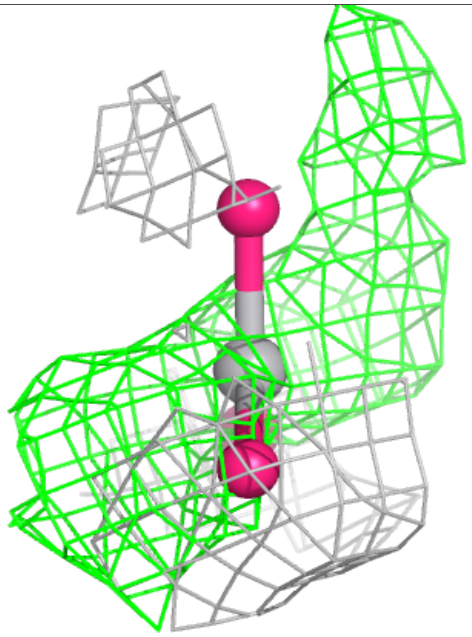


Electron density around VN4 A 1002:

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

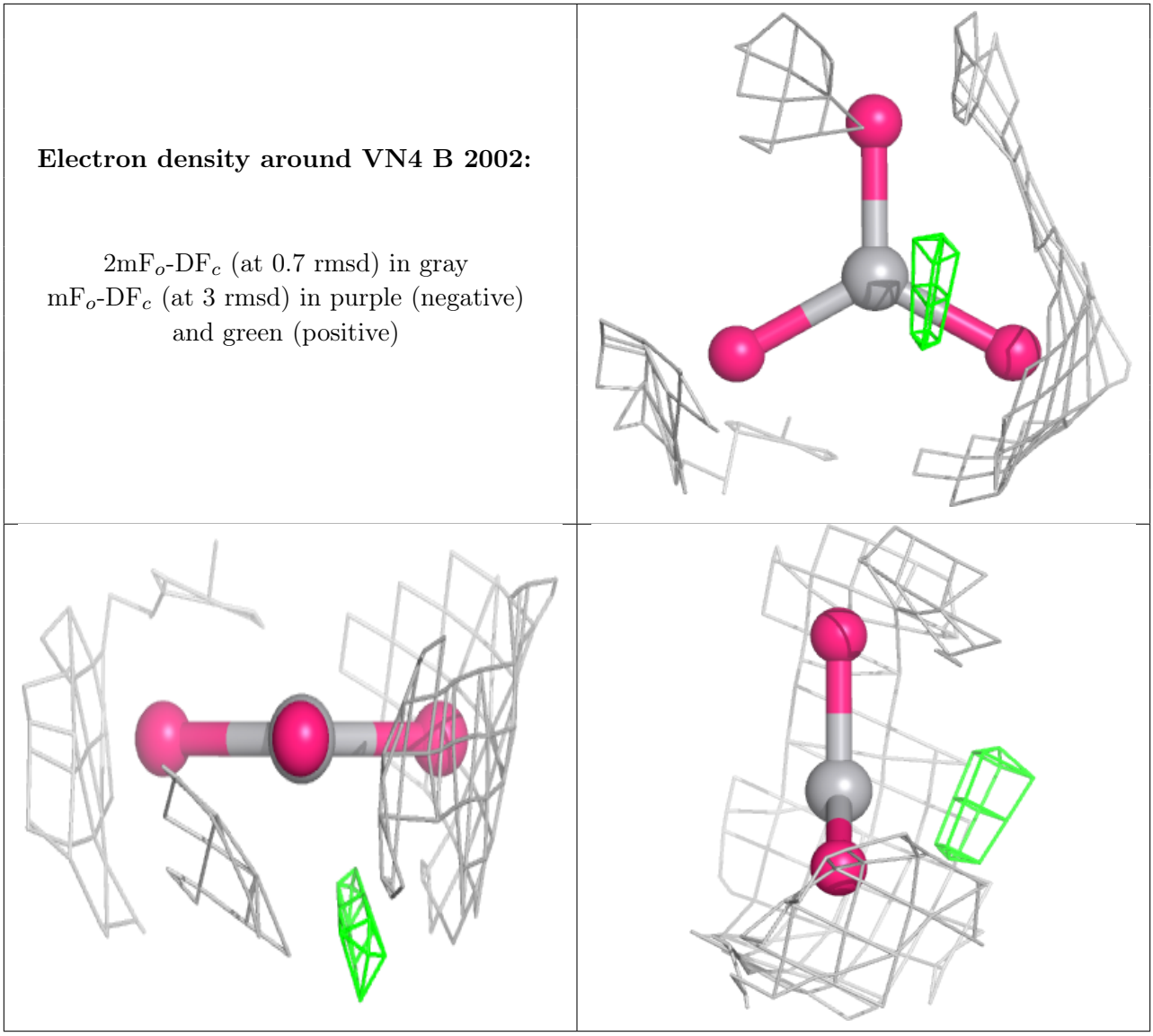






Electron density around VN4 B 2002:

$2mF_o$-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.