



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 04:57 pm BST

PDB ID : 2C88  
Title : Crystal Structure Of (SR) Calcium-ATPase E2(Tg):AMPPCP form  
Authors : Jensen, A.M.; Sorensen, T.L.; Olesen, C.; Moller, J.V.; Nissen, P.  
Deposited on : 2005-12-02  
Resolution : 3.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

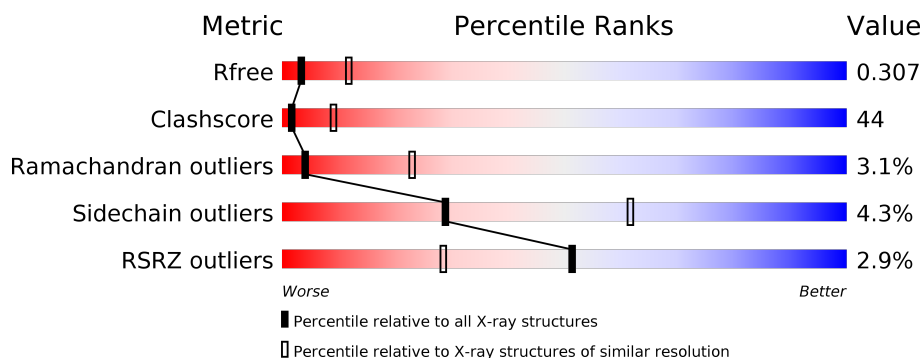
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	994	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACP	A	1996	-	-	-	X
4	MG	A	1997	-	-	-	X

## 2 Entry composition [i](#)

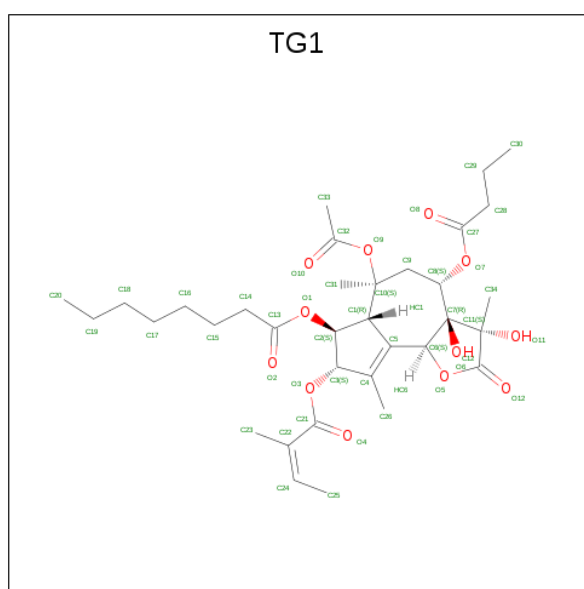
There are 5 unique types of molecules in this entry. The entry contains 7750 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATPASE1 ISOFORM SERCA1A.

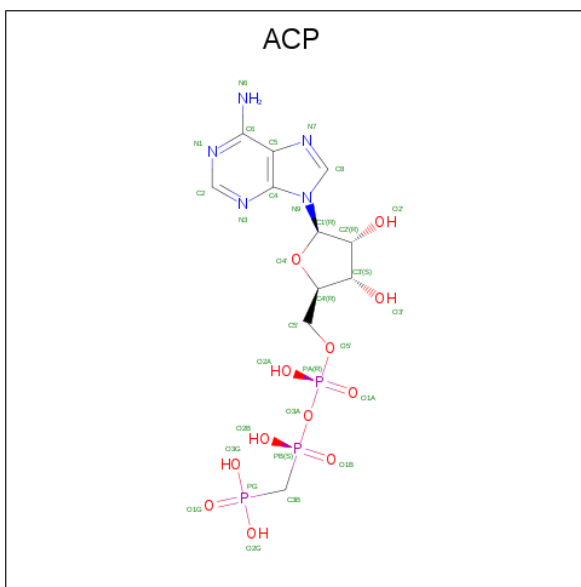
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

- Molecule 2 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)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (three-letter code: TG1) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>12</sub>).



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

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

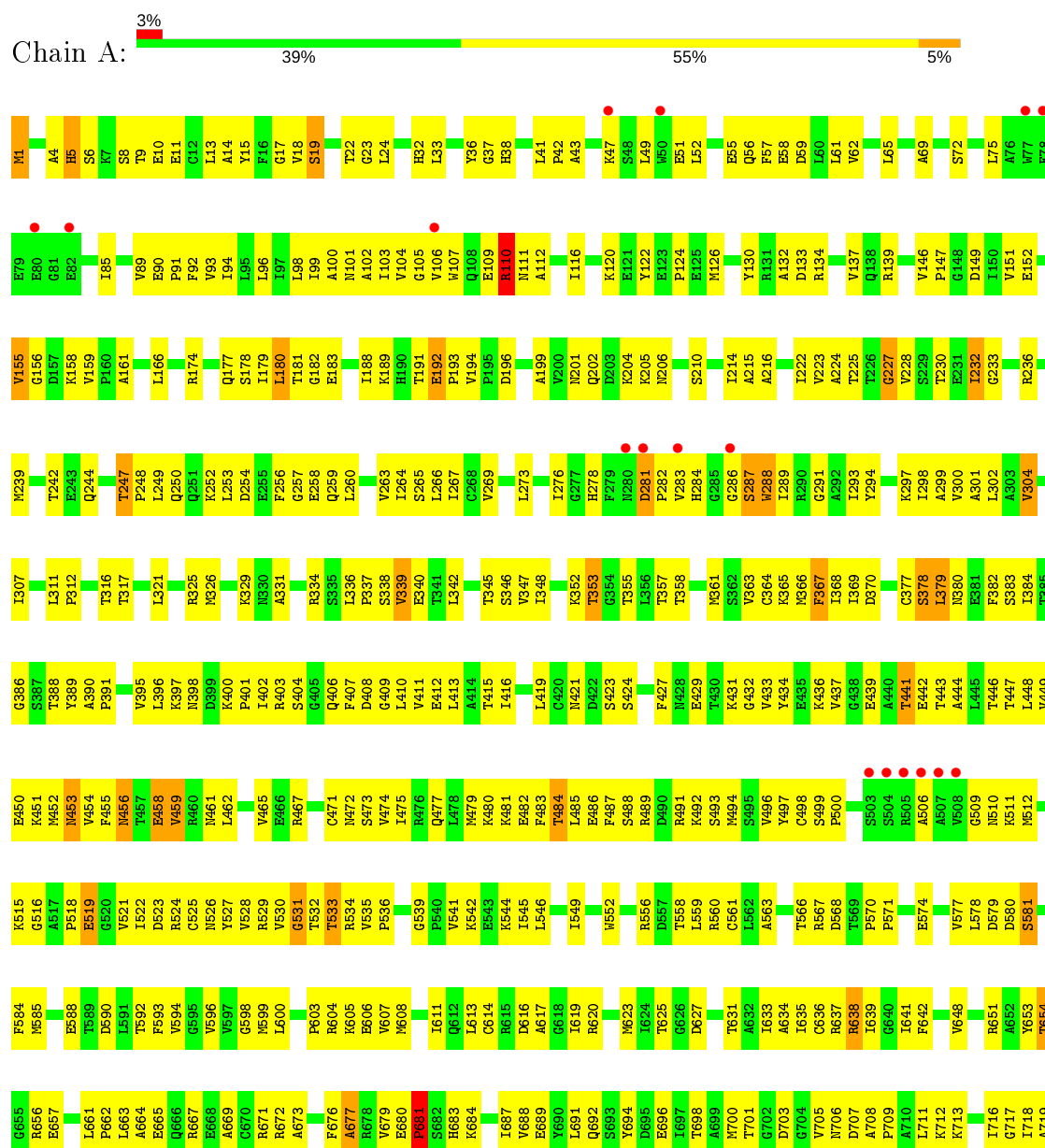
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

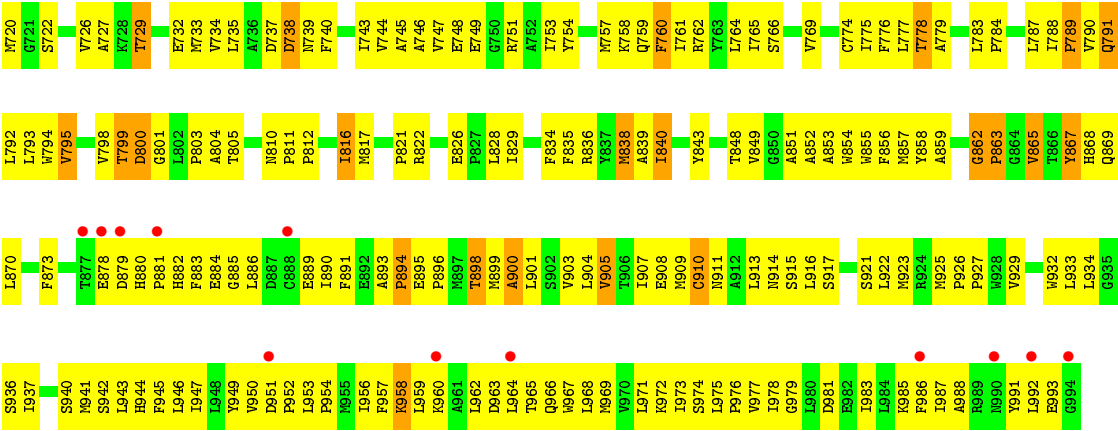
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ATPASE1 ISO-FORM SERCA1A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.53 Å   71.53 Å   590.22 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	14.99 – 3.10 41.72 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (14.99-3.10) 99.7 (41.72-2.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.90 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.261   ,   0.310 0.258   ,   0.307	Depositor DCC
$R_{free}$ test set	1115 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.9	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, ACP, TG1

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	0.48	1/7812 (0.0%)	0.73	4/10592 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	TRP	CB-CG	8.04	1.64	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ARG	NE-CZ-NH2	8.25	124.42	120.30
1	A	1	MET	CA-CB-CG	6.19	123.83	113.30
1	A	110	ARG	CG-CD-NE	-5.80	99.62	111.80
1	A	581	SER	N-CA-C	5.10	124.78	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7671	0	7764	685	0
2	A	46	0	50	4	0
3	A	31	0	14	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	1	0	0	0	0
All	All	7750	0	7828	685	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 44.

All (685) 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:530:VAL:HG23	1:A:533:THR:HG23	1.32	1.05
1:A:334:ARG:HH12	1:A:729:THR:HA	1.22	1.04
1:A:100:ALA:HA	1:A:103:ILE:HD12	1.41	0.99
1:A:247:THR:HG22	1:A:250:GLN:H	1.27	0.99
1:A:898:THR:HG22	1:A:958:LYS:HB2	1.41	0.99
1:A:700:MET:HE3	1:A:701:THR:H	1.28	0.98
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.45	0.98
1:A:248:PRO:HG2	1:A:340:GLU:OE2	1.62	0.97
1:A:485:LEU:HD13	1:A:584:PHE:HD1	1.26	0.96
1:A:436:LYS:HG3	1:A:443:THR:HG21	1.47	0.96
1:A:458:GLU:O	1:A:459:VAL:HG22	1.65	0.96
1:A:342:LEU:O	1:A:345:THR:HG23	1.66	0.93
1:A:865:VAL:HG11	1:A:869:GLN:HB2	1.49	0.93
1:A:247:THR:HG22	1:A:250:GLN:HG3	1.51	0.92
1:A:334:ARG:NH1	1:A:729:THR:HA	1.85	0.91
1:A:901:LEU:HD22	1:A:958:LYS:HZ1	1.38	0.89
1:A:106:VAL:O	1:A:110:ARG:HB2	1.72	0.89
1:A:281:ASP:OD1	1:A:282:PRO:HD3	1.73	0.89
1:A:485:LEU:HD22	1:A:584:PHE:HE1	1.32	0.89
1:A:895:GLU:HA	1:A:898:THR:HG23	1.55	0.88
1:A:606:GLU:CD	1:A:606:GLU:H	1.76	0.88
1:A:485:LEU:HD22	1:A:584:PHE:CE1	2.08	0.88
1:A:397:LYS:O	1:A:400:LYS:HG2	1.74	0.87
1:A:247:THR:CG2	1:A:250:GLN:HG3	2.05	0.87
1:A:484:THR:HB	1:A:496:VAL:HG12	1.55	0.87
1:A:680:GLU:H	1:A:683:HIS:HD2	1.21	0.87
1:A:254:ASP:O	1:A:258:GLU:HG2	1.75	0.87
1:A:247:THR:HG23	1:A:340:GLU:OE1	1.75	0.86
1:A:895:GLU:HA	1:A:898:THR:CG2	2.05	0.85
1:A:485:LEU:HD13	1:A:584:PHE:CD1	2.12	0.85
1:A:748:GLU:HG3	1:A:817:MET:HE3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:THR:HG22	1:A:657:GLU:HG3	1.56	0.84
1:A:298:ILE:CD1	1:A:779:ALA:HB2	2.07	0.84
1:A:388:THR:HG22	1:A:390:ALA:H	1.43	0.84
1:A:99:ILE:HG22	1:A:103:ILE:HD11	1.59	0.83
1:A:759:GLN:HE22	1:A:762:ARG:HH11	1.22	0.83
1:A:62:VAL:HG23	1:A:98:LEU:HD22	1.60	0.83
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.09	0.83
1:A:439:GLU:O	1:A:443:THR:HG22	1.77	0.83
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.61	0.83
1:A:352:LYS:HB2	1:A:625:THR:HG22	1.62	0.82
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.44	0.82
1:A:944:HIS:O	1:A:947:ILE:HG12	1.79	0.82
1:A:560:ARG:NH2	3:A:1996:ACP:H8	1.93	0.82
1:A:865:VAL:HG11	1:A:869:GLN:CB	2.10	0.81
1:A:879:ASP:O	1:A:882:HIS:HB3	1.80	0.81
1:A:59:ASP:HB3	1:A:62:VAL:HG12	1.59	0.81
1:A:909:MET:HE3	1:A:937:ILE:HA	1.61	0.81
1:A:950:VAL:CG1	1:A:952:PRO:HD2	2.11	0.81
1:A:950:VAL:HG13	1:A:952:PRO:HD2	1.62	0.80
1:A:521:VAL:HG21	1:A:563:ALA:HB3	1.62	0.80
1:A:179:ILE:HD12	1:A:180:LEU:HD23	1.64	0.80
1:A:471:CYS:O	1:A:474:VAL:HG22	1.83	0.79
1:A:298:ILE:HD11	1:A:779:ALA:HB2	1.63	0.79
1:A:301:ALA:HA	1:A:789:PRO:HG3	1.63	0.79
1:A:795:VAL:HA	1:A:799:THR:OG1	1.81	0.78
1:A:202:GLN:HB3	1:A:489:ARG:HH21	1.48	0.78
1:A:651:ARG:HH11	1:A:651:ARG:HG2	1.48	0.78
1:A:527:TYR:HB2	1:A:592:THR:HG22	1.65	0.78
1:A:122:TYR:O	1:A:158:LYS:HD3	1.84	0.78
1:A:227:GLY:O	1:A:230:THR:HG22	1.85	0.77
1:A:99:ILE:O	1:A:103:ILE:HG13	1.85	0.76
1:A:680:GLU:N	1:A:683:HIS:HD2	1.84	0.76
1:A:921:SER:OG	1:A:923:MET:HG2	1.85	0.76
1:A:133:ASP:O	1:A:134:ARG:HG3	1.87	0.75
1:A:458:GLU:HG2	1:A:459:VAL:N	2.01	0.75
1:A:828:LEU:HD12	2:A:1995:TG1:H302	1.66	0.75
1:A:436:LYS:CG	1:A:443:THR:HG21	2.16	0.75
1:A:531:GLY:O	1:A:533:THR:HG22	1.86	0.75
1:A:654:THR:CG2	1:A:657:GLU:HG3	2.17	0.74
1:A:93:VAL:HA	1:A:96:LEU:HD12	1.67	0.74
1:A:483:PHE:HE1	1:A:485:LEU:HD21	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ARG:O	1:A:840:ILE:HG12	1.86	0.74
1:A:92:PHE:CE2	1:A:96:LEU:HD11	2.22	0.74
1:A:431:LYS:O	1:A:433:VAL:HG23	1.87	0.74
1:A:177:GLN:HE22	1:A:189:LYS:NZ	1.86	0.73
1:A:458:GLU:CG	1:A:459:VAL:H	1.99	0.73
1:A:700:MET:HE3	1:A:701:THR:N	2.03	0.73
1:A:458:GLU:HG2	1:A:459:VAL:H	1.54	0.73
1:A:526:ASN:HD22	1:A:590:ASP:HA	1.52	0.73
1:A:758:LYS:HA	1:A:761:ILE:HD12	1.71	0.72
1:A:453:ASN:HB3	1:A:471:CYS:SG	2.30	0.72
1:A:89:VAL:O	1:A:93:VAL:HG23	1.90	0.72
1:A:631:THR:O	1:A:635:ILE:HG13	1.89	0.72
1:A:901:LEU:HD22	1:A:958:LYS:NZ	2.04	0.72
1:A:680:GLU:H	1:A:683:HIS:CD2	2.07	0.72
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.30	0.72
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.71	0.71
1:A:317:THR:O	1:A:321:LEU:HG	1.89	0.71
1:A:4:ALA:O	1:A:5:HIS:HB3	1.89	0.71
1:A:521:VAL:HG23	1:A:522:ILE:N	2.05	0.71
1:A:862:GLY:H	1:A:863:PRO:HD3	1.55	0.71
1:A:448:LEU:O	1:A:452:MET:HG2	1.90	0.71
1:A:352:LYS:CB	1:A:625:THR:HG22	2.19	0.71
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.72	0.71
1:A:720:MET:HB3	1:A:738:ASP:OD1	1.90	0.71
1:A:201:ASN:HA	1:A:204:LYS:HG3	1.71	0.71
1:A:248:PRO:O	1:A:252:LYS:HG3	1.91	0.71
1:A:900:ALA:O	1:A:903:VAL:HG12	1.91	0.70
1:A:879:ASP:HB3	1:A:882:HIS:CB	2.20	0.70
1:A:348:ILE:HD13	1:A:743:ILE:HG21	1.72	0.70
1:A:962:LEU:HB3	1:A:966:GLN:HG3	1.73	0.70
1:A:180:LEU:HA	1:A:705:VAL:HG12	1.72	0.69
1:A:368:ILE:HD13	1:A:410:LEU:HD23	1.74	0.69
1:A:436:LYS:HG3	1:A:443:THR:CG2	2.22	0.69
1:A:857:MET:O	1:A:858:TYR:HB2	1.91	0.69
1:A:286:GLY:HA2	1:A:288:TRP:CE3	2.28	0.69
1:A:252:LYS:HE2	1:A:826:GLU:O	1.92	0.69
1:A:560:ARG:HH21	3:A:1996:ACP:H3'	1.57	0.68
1:A:124:PRO:HB3	1:A:158:LYS:HD2	1.76	0.68
1:A:880:HIS:O	1:A:884:GLU:HB2	1.94	0.68
1:A:654:THR:HG22	1:A:657:GLU:H	1.59	0.68
1:A:945:PHE:HD1	1:A:949:TYR:HE2	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ARG:HB2	1:A:216:ALA:H	1.58	0.67
1:A:607:VAL:O	1:A:611:ILE:HG12	1.93	0.67
1:A:909:MET:HE3	1:A:937:ILE:HG23	1.76	0.67
1:A:577:VAL:HG12	1:A:579:ASP:OD1	1.95	0.67
1:A:47:LYS:HB3	1:A:51:GLU:CB	2.25	0.67
1:A:43:ALA:HA	1:A:120:LYS:NZ	2.10	0.67
1:A:654:THR:HG22	1:A:657:GLU:CG	2.24	0.67
1:A:909:MET:CE	1:A:937:ILE:HA	2.24	0.67
1:A:851:ALA:O	1:A:854:TRP:HB3	1.95	0.66
1:A:950:VAL:O	1:A:954:PRO:HG2	1.94	0.66
1:A:14:ALA:O	1:A:17:GLY:N	2.28	0.66
1:A:487:PHE:CE1	1:A:492:LYS:HA	2.31	0.66
1:A:288:TRP:HD1	1:A:289:ILE:HG23	1.60	0.66
1:A:174:ARG:NE	1:A:188:ILE:HG12	2.11	0.66
1:A:49:LEU:HA	1:A:52:LEU:HD12	1.78	0.66
1:A:788:ILE:HG23	1:A:789:PRO:HD2	1.77	0.66
1:A:751:ARG:HH21	1:A:821:PRO:HA	1.60	0.66
1:A:458:GLU:O	1:A:459:VAL:CG2	2.43	0.65
1:A:748:GLU:HA	1:A:817:MET:HE1	1.78	0.65
1:A:452:MET:HG3	1:A:452:MET:O	1.95	0.65
1:A:485:LEU:HB3	1:A:584:PHE:CD1	2.31	0.65
1:A:397:LYS:HB3	1:A:402:ILE:HD11	1.78	0.65
1:A:47:LYS:HB3	1:A:51:GLU:HB2	1.78	0.65
1:A:161:ALA:HA	1:A:210:SER:HB2	1.78	0.65
1:A:522:ILE:HG22	1:A:542:LYS:HE3	1.78	0.65
1:A:278:HIS:O	1:A:282:PRO:HG2	1.97	0.65
1:A:530:VAL:HG23	1:A:533:THR:CG2	2.18	0.65
1:A:848:THR:HA	1:A:903:VAL:HG11	1.77	0.65
1:A:901:LEU:CD2	1:A:958:LYS:HZ1	2.07	0.65
1:A:909:MET:HE1	1:A:940:SER:HB2	1.78	0.65
1:A:535:VAL:HG13	1:A:536:PRO:HD2	1.78	0.65
1:A:69:ALA:HB2	1:A:94:ILE:HG21	1.78	0.65
1:A:895:GLU:CA	1:A:898:THR:HG23	2.26	0.65
1:A:288:TRP:CD1	1:A:289:ILE:HG23	2.32	0.64
1:A:852:ALA:HB2	1:A:900:ALA:HB2	1.80	0.64
1:A:680:GLU:HB3	1:A:681:PRO:CD	2.26	0.64
1:A:23:GLY:HA3	1:A:130:TYR:O	1.98	0.64
1:A:446:THR:O	1:A:449:VAL:HG22	1.96	0.64
1:A:521:VAL:HG23	1:A:522:ILE:H	1.62	0.64
1:A:688:VAL:O	1:A:692:GLN:HG3	1.97	0.64
1:A:927:PRO:HB2	1:A:934:LEU:HD21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASN:HD22	1:A:382:PHE:HE2	1.42	0.64
1:A:968:LEU:O	1:A:972:LYS:HG2	1.97	0.64
1:A:916:LEU:HD11	1:A:933:LEU:HD23	1.79	0.63
1:A:631:THR:HG22	1:A:635:ILE:HD11	1.80	0.63
1:A:352:LYS:HE2	1:A:627:ASP:OD2	1.98	0.63
1:A:244:GLN:CD	1:A:244:GLN:H	2.02	0.63
1:A:521:VAL:CG2	1:A:563:ALA:HB3	2.28	0.63
1:A:581:SER:HA	1:A:584:PHE:CE2	2.33	0.63
1:A:879:ASP:HB3	1:A:882:HIS:HB3	1.80	0.63
1:A:415:THR:HA	1:A:475:ILE:HG21	1.80	0.63
1:A:535:VAL:CG1	1:A:536:PRO:HD2	2.28	0.63
1:A:648:VAL:O	1:A:648:VAL:HG12	1.99	0.62
1:A:458:GLU:CG	1:A:459:VAL:N	2.62	0.62
1:A:483:PHE:CE1	1:A:485:LEU:HD21	2.34	0.62
1:A:491:ARG:NE	1:A:588:GLU:OE1	2.24	0.62
1:A:708:ALA:N	1:A:709:PRO:HD2	2.13	0.62
1:A:751:ARG:HH21	1:A:821:PRO:CA	2.12	0.62
1:A:603:PRO:HG2	1:A:638:ARG:HD3	1.79	0.62
1:A:450:GLU:OE1	1:A:471:CYS:HB2	2.00	0.62
1:A:654:THR:HA	1:A:677:ALA:HB3	1.82	0.61
1:A:979:GLY:O	1:A:983:ILE:HG13	1.99	0.61
1:A:500:PRO:HG3	1:A:506:ALA:HA	1.82	0.61
1:A:926:PRO:HG2	1:A:929:VAL:HG23	1.81	0.61
1:A:474:VAL:HG23	1:A:475:ILE:N	2.15	0.61
1:A:969:MET:O	1:A:973:ILE:HG13	2.00	0.61
1:A:651:ARG:HG2	1:A:651:ARG:NH1	2.16	0.61
1:A:179:ILE:CD1	1:A:180:LEU:HD23	2.31	0.60
1:A:19:SER:OG	1:A:22:THR:HB	2.02	0.60
1:A:312:PRO:O	1:A:316:THR:HG23	2.01	0.60
1:A:879:ASP:CB	1:A:882:HIS:HB3	2.31	0.60
1:A:895:GLU:N	1:A:896:PRO:HD2	2.16	0.60
1:A:751:ARG:HD2	1:A:817:MET:CE	2.31	0.60
1:A:281:ASP:H	1:A:282:PRO:CD	2.14	0.60
1:A:366:MET:HE2	1:A:384:ILE:HD11	1.84	0.60
1:A:391:PRO:HD2	1:A:434:TYR:CE2	2.35	0.60
1:A:480:LYS:N	1:A:499:SER:O	2.33	0.60
1:A:679:VAL:HG13	1:A:683:HIS:CB	2.31	0.60
1:A:963:ASP:HA	1:A:967:TRP:HB2	1.84	0.60
1:A:423:SER:OG	1:A:442:GLU:HB2	2.00	0.60
1:A:593:PHE:HZ	1:A:596:VAL:HG13	1.66	0.59
1:A:933:LEU:O	1:A:937:ILE:HG13	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ASP:O	1:A:411:VAL:HG22	2.00	0.59
1:A:298:ILE:HD13	1:A:779:ALA:HB2	1.82	0.59
1:A:404:SER:OG	1:A:452:MET:HB2	2.03	0.59
1:A:166:LEU:HD11	1:A:222:ILE:HB	1.84	0.59
1:A:654:THR:CG2	1:A:657:GLU:H	2.14	0.59
1:A:177:GLN:HE22	1:A:189:LYS:HZ1	1.49	0.59
1:A:532:THR:HG23	1:A:532:THR:O	2.02	0.59
1:A:901:LEU:HD13	1:A:958:LYS:HZ1	1.67	0.59
1:A:33:LEU:HD11	1:A:38:HIS:ND1	2.18	0.59
1:A:106:VAL:O	1:A:110:ARG:CB	2.49	0.58
1:A:748:GLU:HA	1:A:817:MET:CE	2.32	0.58
1:A:59:ASP:OD2	1:A:61:LEU:HB2	2.02	0.58
1:A:104:VAL:HG12	1:A:105:GLY:N	2.18	0.58
1:A:639:ILE:HD11	1:A:641:ILE:HG12	1.85	0.58
1:A:284:HIS:ND1	1:A:284:HIS:O	2.35	0.58
1:A:577:VAL:HB	1:A:580:ASP:OD1	2.03	0.58
1:A:884:GLU:O	1:A:886:LEU:N	2.35	0.58
1:A:950:VAL:CG1	1:A:951:ASP:N	2.67	0.58
1:A:122:TYR:HE2	1:A:726:VAL:HG21	1.68	0.58
1:A:474:VAL:CG2	1:A:475:ILE:N	2.66	0.58
1:A:22:THR:HG22	1:A:132:ALA:HB2	1.86	0.58
1:A:527:TYR:O	1:A:592:THR:HA	2.03	0.58
1:A:879:ASP:HB3	1:A:882:HIS:HB2	1.85	0.58
1:A:855:TRP:CZ2	1:A:895:GLU:HG3	2.38	0.58
1:A:498:CYS:O	1:A:510:ASN:HA	2.04	0.57
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.86	0.57
1:A:398:ASN:HD22	1:A:400:LYS:NZ	2.02	0.57
1:A:671:ARG:HB3	1:A:694:TYR:CE2	2.39	0.57
1:A:155:VAL:O	1:A:214:ILE:O	2.22	0.57
1:A:192:GLU:OE1	1:A:580:ASP:HB2	2.04	0.57
1:A:110:ARG:NH1	1:A:110:ARG:HG2	2.18	0.57
1:A:10:GLU:N	1:A:10:GLU:OE1	2.36	0.57
1:A:151:VAL:HG12	1:A:152:GLU:N	2.20	0.57
1:A:242:THR:HG21	1:A:712:LYS:HD3	1.87	0.57
1:A:178:SER:O	1:A:182:GLY:N	2.37	0.57
1:A:898:THR:HB	1:A:958:LYS:HG3	1.87	0.56
1:A:75:LEU:HD13	1:A:297:LYS:HB3	1.86	0.56
1:A:100:ALA:HA	1:A:103:ILE:CD1	2.26	0.56
1:A:247:THR:HG23	1:A:249:LEU:H	1.70	0.56
1:A:459:VAL:HA	1:A:462:LEU:HG	1.87	0.56
1:A:926:PRO:O	1:A:929:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:LEU:O	1:A:957:PHE:HD2	1.88	0.56
1:A:242:THR:CG2	1:A:712:LYS:HD3	2.36	0.56
1:A:389:TYR:CE2	1:A:436:LYS:HB2	2.41	0.56
1:A:334:ARG:HH12	1:A:729:THR:CA	2.07	0.56
1:A:559:LEU:HD23	1:A:600:LEU:HB2	1.87	0.56
1:A:181:THR:OG1	1:A:183:GLU:HG2	2.05	0.56
1:A:147:PRO:HA	1:A:223:VAL:CG1	2.34	0.56
1:A:342:LEU:CD2	1:A:733:MET:HE1	2.36	0.56
1:A:676:PHE:CE2	1:A:687:ILE:HD13	2.41	0.56
1:A:72:SER:OG	1:A:91:PRO:HD3	2.05	0.56
1:A:300:VAL:O	1:A:304:VAL:HG13	2.06	0.56
1:A:429:GLU:CD	1:A:429:GLU:N	2.59	0.56
1:A:909:MET:HE3	1:A:937:ILE:CA	2.35	0.56
1:A:6:SER:HA	1:A:194:VAL:O	2.06	0.55
1:A:411:VAL:CA	1:A:454:VAL:HG11	2.36	0.55
1:A:558:THR:HG22	1:A:634:ALA:HB1	1.87	0.55
1:A:267:ILE:HD11	2:A:1995:TG1:H182	1.88	0.55
1:A:788:ILE:HG22	1:A:790:VAL:HG23	1.87	0.55
1:A:183:GLU:HG3	1:A:183:GLU:O	2.07	0.55
1:A:47:LYS:HA	1:A:51:GLU:OE1	2.07	0.55
1:A:75:LEU:HD22	1:A:293:ILE:HG13	1.87	0.55
1:A:788:ILE:CG2	1:A:790:VAL:HG23	2.37	0.55
1:A:18:VAL:HG22	1:A:19:SER:N	2.21	0.55
1:A:55:GLU:HA	1:A:58:GLU:HB2	1.87	0.55
1:A:174:ARG:HB2	1:A:216:ALA:N	2.22	0.55
1:A:835:PHE:O	1:A:838:MET:HB3	2.06	0.55
1:A:102:ALA:O	1:A:106:VAL:HG12	2.06	0.55
1:A:202:GLN:HB3	1:A:489:ARG:NH2	2.20	0.55
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.42	0.55
1:A:347:VAL:HG22	1:A:620:ARG:HB3	1.87	0.55
1:A:286:GLY:O	1:A:287:SER:CB	2.55	0.55
1:A:348:ILE:HD13	1:A:743:ILE:CG2	2.37	0.55
1:A:370:ASP:HB3	1:A:378:SER:O	2.06	0.55
1:A:515:LYS:HE3	3:A:1996:ACP:N1	2.22	0.55
1:A:455:PHE:O	1:A:456:ASN:C	2.44	0.55
1:A:895:GLU:O	1:A:898:THR:HG23	2.06	0.55
1:A:177:GLN:NE2	1:A:189:LYS:NZ	2.54	0.54
1:A:530:VAL:O	1:A:531:GLY:O	2.24	0.54
1:A:205:LYS:NZ	1:A:488:SER:HB3	2.22	0.54
1:A:286:GLY:HA2	1:A:288:TRP:CZ3	2.42	0.54
1:A:411:VAL:CB	1:A:454:VAL:HG11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HA	1:A:120:LYS:HZ1	1.70	0.54
1:A:855:TRP:HE3	1:A:856:PHE:CD1	2.26	0.54
1:A:161:ALA:CA	1:A:210:SER:HB2	2.37	0.54
1:A:581:SER:HA	1:A:584:PHE:CD2	2.43	0.54
1:A:764:LEU:HD21	1:A:804:ALA:HB2	1.90	0.54
1:A:408:ASP:O	1:A:411:VAL:N	2.40	0.54
1:A:436:LYS:CD	1:A:443:THR:HG21	2.37	0.54
1:A:975:LEU:HB2	1:A:976:PRO:HD3	1.89	0.54
1:A:367:PHE:C	1:A:367:PHE:CD1	2.81	0.54
1:A:661:LEU:HD13	1:A:665:GLU:HG3	1.88	0.54
1:A:882:HIS:CD2	1:A:883:PHE:HD2	2.26	0.54
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.38	0.54
1:A:940:SER:O	1:A:943:LEU:HB2	2.08	0.54
1:A:642:PHE:CZ	1:A:648:VAL:HG13	2.43	0.54
1:A:653:TYR:CE2	1:A:669:ALA:HB1	2.43	0.54
1:A:408:ASP:O	1:A:409:GLY:C	2.45	0.53
1:A:639:ILE:HD11	1:A:641:ILE:CG1	2.38	0.53
1:A:524:ARG:HD2	1:A:588:GLU:O	2.08	0.53
1:A:909:MET:CE	1:A:940:SER:HB2	2.37	0.53
1:A:388:THR:HG22	1:A:390:ALA:N	2.20	0.53
1:A:5:HIS:HE1	1:A:196:ASP:O	1.91	0.53
1:A:1:MET:HB3	1:A:225:THR:HG22	1.90	0.53
1:A:230:THR:O	1:A:233:GLY:N	2.42	0.53
1:A:265:SER:O	1:A:269:VAL:HG23	2.07	0.53
1:A:707:ASP:O	1:A:711:LEU:HG	2.08	0.53
1:A:748:GLU:CG	1:A:817:MET:HE3	2.36	0.53
1:A:901:LEU:HD13	1:A:958:LYS:NZ	2.23	0.53
1:A:751:ARG:HD2	1:A:817:MET:HE1	1.90	0.53
1:A:909:MET:CE	1:A:937:ILE:HG23	2.38	0.53
1:A:411:VAL:HB	1:A:454:VAL:HG11	1.90	0.53
1:A:963:ASP:O	1:A:964:LEU:HB2	2.07	0.53
1:A:369:ILE:HG22	1:A:530:VAL:HG12	1.91	0.53
1:A:865:VAL:HG11	1:A:869:GLN:CG	2.39	0.53
1:A:421:ASN:ND2	1:A:446:THR:HG23	2.24	0.53
1:A:560:ARG:CZ	3:A:1996:ACP:H8	2.39	0.53
1:A:260:LEU:O	1:A:264:ILE:HG13	2.09	0.53
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.91	0.53
1:A:857:MET:O	1:A:858:TYR:CB	2.58	0.53
1:A:529:ARG:HG3	1:A:533:THR:O	2.09	0.52
1:A:759:GLN:NE2	1:A:762:ARG:HH11	2.01	0.52
1:A:812:PRO:HB2	1:A:816:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:ILE:O	1:A:843:TYR:HB3	2.09	0.52
1:A:945:PHE:CD1	1:A:949:TYR:HE2	2.24	0.52
1:A:671:ARG:HB3	1:A:694:TYR:CD2	2.44	0.52
1:A:766:SER:O	1:A:769:VAL:HB	2.10	0.52
1:A:281:ASP:N	1:A:282:PRO:CD	2.71	0.52
1:A:568:ASP:OD2	1:A:592:THR:HG21	2.09	0.52
1:A:59:ASP:HB3	1:A:62:VAL:CG1	2.35	0.52
1:A:943:LEU:O	1:A:946:LEU:HB3	2.09	0.52
1:A:950:VAL:HG12	1:A:951:ASP:N	2.25	0.52
1:A:342:LEU:HD22	1:A:733:MET:HE1	1.92	0.52
1:A:458:GLU:C	1:A:459:VAL:HG13	2.30	0.52
1:A:485:LEU:O	1:A:491:ARG:NH2	2.43	0.52
1:A:427:PHE:HD2	1:A:465:VAL:HG22	1.74	0.52
1:A:449:VAL:CG2	1:A:472:ASN:ND2	2.73	0.52
1:A:925:MET:CE	1:A:929:VAL:HG11	2.40	0.52
1:A:962:LEU:HB3	1:A:966:GLN:CG	2.39	0.52
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.10	0.52
1:A:346:SER:OG	1:A:696:GLU:HG2	2.10	0.52
1:A:512:MET:HE3	1:A:570:PRO:HB2	1.91	0.52
1:A:159:VAL:O	1:A:210:SER:HA	2.10	0.52
1:A:8:SER:OG	1:A:11:GLU:HG3	2.10	0.51
1:A:793:LEU:O	1:A:794:TRP:C	2.47	0.51
1:A:361:MET:HB3	1:A:599:MET:HE2	1.92	0.51
1:A:691:LEU:O	1:A:696:GLU:HB2	2.10	0.51
1:A:453:ASN:O	1:A:453:ASN:OD1	2.28	0.51
1:A:408:ASP:HA	1:A:411:VAL:HG13	1.91	0.51
1:A:411:VAL:HG12	1:A:454:VAL:HG13	1.91	0.51
1:A:398:ASN:HD22	1:A:400:LYS:HZ2	1.58	0.51
1:A:47:LYS:HB3	1:A:51:GLU:HB3	1.91	0.51
1:A:526:ASN:ND2	1:A:590:ASP:HA	2.23	0.51
1:A:500:PRO:HD3	1:A:509:GLY:HA2	1.92	0.51
1:A:527:TYR:HD2	1:A:592:THR:HG22	1.76	0.51
1:A:441:THR:HG21	1:A:560:ARG:HH12	1.76	0.51
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.91	0.51
1:A:239:MET:O	1:A:242:THR:HG22	2.11	0.51
1:A:719:ALA:HB3	1:A:734:VAL:HG22	1.93	0.51
1:A:407:PHE:O	1:A:411:VAL:HG13	2.10	0.50
1:A:890:ILE:O	1:A:893:ALA:HB2	2.10	0.50
1:A:733:MET:HG2	1:A:734:VAL:N	2.26	0.50
1:A:829:ILE:HG21	2:A:1995:TG1:H333	1.92	0.50
1:A:870:LEU:O	1:A:870:LEU:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:THR:HA	1:A:958:LYS:CE	2.41	0.50
1:A:411:VAL:O	1:A:415:THR:HG23	2.12	0.50
1:A:608:MET:SD	1:A:639:ILE:HA	2.51	0.50
1:A:467:ARG:NH1	1:A:467:ARG:O	2.44	0.50
1:A:489:ARG:O	1:A:492:LYS:HE3	2.11	0.50
1:A:744:VAL:O	1:A:745:ALA:C	2.49	0.50
1:A:358:THR:O	1:A:358:THR:HG22	2.11	0.50
1:A:69:ALA:HB2	1:A:94:ILE:CG2	2.41	0.50
1:A:901:LEU:C	1:A:901:LEU:HD23	2.32	0.50
1:A:969:MET:HE3	1:A:972:LYS:HG3	1.94	0.50
1:A:24:LEU:HD13	1:A:149:ASP:HA	1.94	0.50
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.42	0.50
1:A:4:ALA:O	1:A:5:HIS:CB	2.59	0.50
1:A:379:LEU:HD22	1:A:544:LYS:HE3	1.93	0.50
1:A:749:GLU:O	1:A:753:ILE:HG12	2.12	0.50
1:A:512:MET:O	1:A:566:THR:HA	2.12	0.50
1:A:703:ASP:O	1:A:727:ALA:HB2	2.12	0.50
1:A:762:ARG:NH2	1:A:828:LEU:O	2.42	0.49
1:A:662:PRO:O	1:A:664:ALA:N	2.45	0.49
1:A:151:VAL:HG21	1:A:223:VAL:HG23	1.92	0.49
1:A:242:THR:HG23	1:A:712:LYS:NZ	2.28	0.49
1:A:482:GLU:HG3	1:A:497:TYR:HD2	1.77	0.49
1:A:913:LEU:HD21	1:A:937:ILE:CD1	2.42	0.49
1:A:479:MET:HA	1:A:500:PRO:HA	1.95	0.49
1:A:605:LYS:HB2	1:A:606:GLU:OE2	2.11	0.49
1:A:421:ASN:HD21	1:A:446:THR:HG23	1.77	0.49
1:A:436:LYS:HG3	1:A:443:THR:CB	2.43	0.49
1:A:574:GLU:OE1	1:A:574:GLU:N	2.44	0.49
1:A:353:THR:HA	1:A:357:THR:OG1	2.13	0.49
1:A:521:VAL:CG2	1:A:522:ILE:N	2.75	0.49
1:A:757:MET:HA	1:A:760:PHE:CE2	2.48	0.49
1:A:843:TYR:CD2	1:A:977:VAL:HG22	2.48	0.49
1:A:894:PRO:O	1:A:898:THR:HG22	2.12	0.49
1:A:788:ILE:HG22	1:A:790:VAL:H	1.78	0.49
1:A:901:LEU:HB3	1:A:958:LYS:HE3	1.94	0.49
1:A:898:THR:CG2	1:A:958:LYS:HB2	2.29	0.48
1:A:180:LEU:O	1:A:706:ASN:ND2	2.46	0.48
1:A:263:VAL:O	1:A:266:LEU:HB2	2.13	0.48
1:A:304:VAL:HG21	1:A:789:PRO:HA	1.94	0.48
1:A:65:LEU:HD21	1:A:307:ILE:HD12	1.95	0.48
1:A:236:ARG:O	1:A:236:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ASN:O	1:A:462:LEU:HD23	2.14	0.48
1:A:530:VAL:CG2	1:A:533:THR:HG23	2.24	0.48
1:A:527:TYR:CD2	1:A:592:THR:HG22	2.48	0.48
1:A:606:GLU:CD	1:A:606:GLU:N	2.56	0.48
1:A:352:LYS:CE	1:A:627:ASP:OD2	2.60	0.48
1:A:441:THR:HG21	1:A:560:ARG:NH1	2.28	0.48
1:A:865:VAL:HG11	1:A:869:GLN:HG2	1.95	0.48
1:A:760:PHE:C	1:A:760:PHE:CD1	2.86	0.48
1:A:971:LEU:HB3	1:A:975:LEU:HD11	1.96	0.48
1:A:116:ILE:HG23	1:A:236:ARG:HG3	1.96	0.48
1:A:47:LYS:HD2	1:A:51:GLU:OE2	2.14	0.48
1:A:411:VAL:HA	1:A:454:VAL:HG21	1.95	0.48
1:A:65:LEU:HG	1:A:307:ILE:CD1	2.43	0.48
1:A:424:SER:O	1:A:437:VAL:HB	2.13	0.48
1:A:449:VAL:HG21	1:A:472:ASN:CG	2.34	0.48
1:A:546:LEU:O	1:A:549:ILE:HB	2.13	0.48
1:A:654:THR:HG23	1:A:656:ARG:H	1.77	0.48
1:A:751:ARG:HD2	1:A:817:MET:HE2	1.96	0.48
1:A:908:GLU:C	1:A:910:CYS:N	2.66	0.48
1:A:388:THR:HG22	1:A:389:TYR:N	2.28	0.47
1:A:325:ARG:NH1	1:A:753:ILE:HD11	2.29	0.47
1:A:57:PHE:HE1	1:A:102:ALA:HB2	1.79	0.47
1:A:740:PHE:O	1:A:743:ILE:HB	2.13	0.47
1:A:856:PHE:HE2	1:A:891:PHE:HD1	1.61	0.47
1:A:259:GLN:O	1:A:260:LEU:C	2.51	0.47
1:A:36:TYR:CG	1:A:147:PRO:HG2	2.50	0.47
1:A:519:GLU:H	1:A:519:GLU:CD	2.17	0.47
1:A:230:THR:HG23	1:A:233:GLY:H	1.79	0.47
1:A:509:GLY:O	1:A:511:LYS:HG2	2.14	0.47
1:A:549:ILE:HD11	1:A:596:VAL:HG11	1.95	0.47
1:A:855:TRP:O	1:A:859:ALA:HB3	2.14	0.47
1:A:85:ILE:HG13	1:A:85:ILE:O	2.14	0.47
1:A:956:ILE:HB	1:A:957:PHE:CD2	2.50	0.47
1:A:959:LEU:HG	1:A:960:LYS:N	2.28	0.47
1:A:895:GLU:C	1:A:898:THR:HG23	2.34	0.47
1:A:338:SER:O	1:A:339:VAL:C	2.53	0.47
1:A:450:GLU:CD	1:A:471:CYS:HB2	2.35	0.47
1:A:518:PRO:HD3	1:A:561:CYS:O	2.14	0.47
1:A:623:MET:SD	1:A:625:THR:CG2	3.03	0.47
1:A:388:THR:CG2	1:A:390:ALA:H	2.22	0.47
1:A:397:LYS:O	1:A:398:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ALA:O	1:A:447:THR:N	2.46	0.47
1:A:521:VAL:HG21	1:A:563:ALA:CB	2.37	0.47
1:A:247:THR:CB	1:A:250:GLN:HG3	2.45	0.47
1:A:363:VAL:HG11	1:A:448:LEU:HD22	1.96	0.47
1:A:465:VAL:O	1:A:465:VAL:HG12	2.14	0.47
1:A:896:PRO:O	1:A:899:MET:HB2	2.14	0.47
1:A:388:THR:C	1:A:390:ALA:H	2.17	0.47
1:A:388:THR:C	1:A:390:ALA:N	2.66	0.47
1:A:735:LEU:HD23	1:A:735:LEU:N	2.28	0.47
1:A:901:LEU:CD1	1:A:958:LYS:HZ1	2.27	0.47
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.50	0.47
1:A:964:LEU:HA	1:A:968:LEU:HG	1.97	0.47
1:A:442:GLU:C	1:A:444:ALA:H	2.18	0.47
1:A:491:ARG:HB2	1:A:585:MET:HG3	1.96	0.47
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.96	0.47
1:A:769:VAL:HA	2:A:1995:TG1:H24	1.96	0.46
1:A:949:TYR:HA	1:A:960:LYS:HE2	1.96	0.46
1:A:18:VAL:CG2	1:A:19:SER:N	2.77	0.46
1:A:249:LEU:O	1:A:253:LEU:HG	2.15	0.46
1:A:619:ILE:CD1	1:A:747:VAL:HG11	2.45	0.46
1:A:65:LEU:CD2	1:A:307:ILE:HD12	2.45	0.46
1:A:950:VAL:O	1:A:954:PRO:CG	2.61	0.46
1:A:492:LYS:O	1:A:493:SER:HB3	2.15	0.46
1:A:639:ILE:CD1	1:A:641:ILE:HG12	2.45	0.46
1:A:32:HIS:HB3	1:A:146:VAL:HG13	1.98	0.46
1:A:345:THR:HG22	1:A:716:ILE:HD13	1.98	0.46
1:A:382:PHE:CZ	1:A:410:LEU:HD11	2.50	0.46
1:A:541:VAL:O	1:A:545:ILE:HG13	2.16	0.46
1:A:109:GLU:O	1:A:112:ALA:HB3	2.16	0.46
1:A:193:PRO:HA	1:A:206:ASN:ND2	2.31	0.46
1:A:865:VAL:CG1	1:A:869:GLN:H	2.28	0.46
1:A:784:PRO:HG3	1:A:873:PHE:CD2	2.51	0.46
1:A:178:SER:C	1:A:180:LEU:N	2.69	0.46
1:A:383:SER:C	1:A:384:ILE:HD12	2.36	0.46
1:A:530:VAL:O	1:A:533:THR:CG2	2.64	0.46
1:A:910:CYS:SG	1:A:978:ILE:HD11	2.55	0.46
1:A:500:PRO:CD	1:A:509:GLY:HA2	2.46	0.46
1:A:898:THR:HA	1:A:958:LYS:HE3	1.97	0.46
1:A:355:THR:HB	1:A:738:ASP:O	2.16	0.46
1:A:530:VAL:O	1:A:530:VAL:HG23	2.15	0.45
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ALA:O	1:A:302:LEU:HB3	2.16	0.45
1:A:534:ARG:HD2	1:A:592:THR:HG21	1.99	0.45
1:A:775:ILE:O	1:A:778:THR:HG22	2.15	0.45
1:A:648:VAL:O	1:A:648:VAL:CG1	2.65	0.45
1:A:122:TYR:HE2	1:A:726:VAL:CG2	2.29	0.45
1:A:329:LYS:HZ2	1:A:749:GLU:HG2	1.81	0.45
1:A:974:SER:C	1:A:976:PRO:HD2	2.36	0.45
1:A:633:ILE:CG2	1:A:637:ARG:NH1	2.80	0.45
1:A:701:THR:HA	1:A:718:ILE:O	2.16	0.45
1:A:792:LEU:O	1:A:795:VAL:HB	2.15	0.45
1:A:944:HIS:HD2	1:A:947:ILE:HD11	1.81	0.45
1:A:971:LEU:HB3	1:A:975:LEU:CD1	2.46	0.45
1:A:442:GLU:C	1:A:444:ALA:N	2.69	0.45
1:A:900:ALA:C	1:A:903:VAL:HG12	2.37	0.45
1:A:151:VAL:CG2	1:A:223:VAL:HG23	2.46	0.45
1:A:1:MET:HA	1:A:224:ALA:O	2.15	0.45
1:A:412:GLU:OE2	1:A:594:VAL:HG11	2.17	0.45
1:A:856:PHE:CZ	1:A:891:PHE:HA	2.52	0.45
1:A:107:TRP:CD1	1:A:111:ASN:ND2	2.85	0.45
1:A:904:LEU:O	1:A:905:VAL:C	2.55	0.45
1:A:951:ASP:O	1:A:954:PRO:HD2	2.16	0.45
1:A:969:MET:HE3	1:A:969:MET:O	2.17	0.45
1:A:987:ILE:HG22	1:A:987:ILE:O	2.17	0.45
1:A:614:CYS:HA	1:A:617:ALA:HB3	1.99	0.45
1:A:106:VAL:HG22	1:A:110:ARG:HD2	1.99	0.45
1:A:338:SER:O	1:A:340:GLU:N	2.49	0.45
1:A:689:GLU:HG3	1:A:713:LYS:HZ2	1.81	0.45
1:A:447:THR:CG2	1:A:451:LYS:HE3	2.47	0.44
1:A:47:LYS:HD2	1:A:51:GLU:CD	2.37	0.44
1:A:331:ALA:HB1	1:A:733:MET:HE2	1.97	0.44
1:A:962:LEU:HG	1:A:965:THR:OG1	2.16	0.44
1:A:397:LYS:HB3	1:A:402:ILE:CD1	2.44	0.44
1:A:402:ILE:HG22	1:A:403:ARG:N	2.33	0.44
1:A:672:ARG:HG3	1:A:673:ALA:N	2.31	0.44
1:A:689:GLU:CG	1:A:713:LYS:NZ	2.81	0.44
1:A:722:SER:OG	1:A:738:ASP:OD2	2.30	0.44
1:A:839:ALA:O	1:A:840:ILE:C	2.56	0.44
1:A:18:VAL:CG2	1:A:24:LEU:HD12	2.47	0.44
1:A:367:PHE:CD2	1:A:596:VAL:HG22	2.52	0.44
1:A:419:LEU:O	1:A:481:LYS:HE3	2.17	0.44
1:A:419:LEU:O	1:A:496:VAL:HG21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:TYR:HB2	1:A:592:THR:CG2	2.43	0.44
1:A:708:ALA:N	1:A:709:PRO:CD	2.80	0.44
1:A:932:TRP:HA	1:A:932:TRP:CE3	2.52	0.44
1:A:13:LEU:HD23	1:A:13:LEU:HA	1.74	0.44
1:A:991:TYR:CE2	1:A:993:GLU:HG3	2.53	0.44
1:A:291:GLY:O	1:A:294:TYR:HB3	2.18	0.44
1:A:449:VAL:HG23	1:A:450:GLU:N	2.33	0.44
1:A:512:MET:CE	1:A:571:PRO:HD2	2.48	0.44
1:A:890:ILE:O	1:A:893:ALA:CB	2.66	0.44
1:A:959:LEU:HG	1:A:960:LYS:H	1.83	0.44
1:A:286:GLY:O	1:A:287:SER:HB3	2.18	0.44
1:A:449:VAL:HG21	1:A:472:ASN:ND2	2.33	0.44
1:A:529:ARG:HG3	1:A:529:ARG:HH11	1.81	0.44
1:A:530:VAL:O	1:A:533:THR:HG23	2.18	0.44
1:A:193:PRO:HA	1:A:206:ASN:HD22	1.82	0.44
1:A:174:ARG:HB3	1:A:215:ALA:HB3	2.00	0.44
1:A:662:PRO:C	1:A:664:ALA:N	2.71	0.44
1:A:800:ASP:O	1:A:803:PRO:HG2	2.18	0.44
1:A:855:TRP:HA	1:A:859:ALA:HB2	2.00	0.44
1:A:395:VAL:O	1:A:396:LEU:HD23	2.18	0.43
1:A:398:ASN:ND2	1:A:400:LYS:NZ	2.65	0.43
1:A:412:GLU:CD	1:A:529:ARG:HE	2.21	0.43
1:A:202:GLN:CB	1:A:489:ARG:HH21	2.25	0.43
1:A:613:LEU:O	1:A:616:ASP:HB2	2.18	0.43
1:A:41:LEU:O	1:A:42:PRO:C	2.57	0.43
1:A:798:VAL:O	1:A:800:ASP:N	2.51	0.43
1:A:880:HIS:N	1:A:881:PRO:HD2	2.33	0.43
1:A:908:GLU:C	1:A:910:CYS:H	2.21	0.43
1:A:61:LEU:HD21	1:A:257:GLY:HA2	2.00	0.43
1:A:523:ASP:C	1:A:525:CYS:H	2.21	0.43
1:A:783:LEU:HD21	1:A:853:ALA:HB2	1.99	0.43
1:A:377:CYS:SG	1:A:541:VAL:HG13	2.58	0.43
1:A:402:ILE:CG2	1:A:403:ARG:N	2.82	0.43
1:A:448:LEU:HD12	1:A:448:LEU:O	2.19	0.43
1:A:473:SER:O	1:A:477:GLN:HG3	2.17	0.43
1:A:415:THR:HG22	1:A:475:ILE:HG23	2.00	0.43
1:A:196:ASP:HB3	1:A:199:ALA:HB2	2.00	0.43
1:A:522:ILE:O	1:A:525:CYS:HB2	2.19	0.43
1:A:882:HIS:CD2	1:A:883:PHE:CD2	3.06	0.43
1:A:101:ASN:O	1:A:104:VAL:HB	2.19	0.43
1:A:273:LEU:O	1:A:276:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:VAL:HG12	1:A:593:PHE:HB3	1.99	0.43
1:A:913:LEU:HD23	1:A:933:LEU:HD21	2.00	0.43
1:A:14:ALA:O	1:A:15:TYR:C	2.57	0.43
1:A:882:HIS:O	1:A:882:HIS:CG	2.70	0.43
1:A:922:LEU:HD23	1:A:922:LEU:HA	1.78	0.43
1:A:33:LEU:O	1:A:37:GLY:N	2.49	0.43
1:A:556:ARG:HG2	1:A:556:ARG:HH11	1.83	0.43
1:A:811:PRO:HA	1:A:812:PRO:HD3	1.85	0.43
1:A:855:TRP:HE3	1:A:856:PHE:HD1	1.65	0.43
1:A:991:TYR:CG	1:A:992:LEU:N	2.86	0.43
1:A:411:VAL:CG2	1:A:412:GLU:N	2.81	0.43
1:A:991:TYR:HE2	1:A:993:GLU:HG3	1.83	0.43
1:A:909:MET:HE3	1:A:937:ILE:CG2	2.48	0.43
1:A:951:ASP:C	1:A:954:PRO:HD2	2.39	0.43
1:A:482:GLU:HG3	1:A:497:TYR:CD2	2.53	0.42
1:A:363:VAL:HG13	1:A:598:GLY:O	2.19	0.42
1:A:865:VAL:HG11	1:A:869:GLN:H	1.83	0.42
1:A:981:ASP:OD2	1:A:985:LYS:HE3	2.19	0.42
1:A:151:VAL:CG1	1:A:152:GLU:N	2.81	0.42
1:A:336:LEU:HB2	1:A:337:PRO:HD3	2.00	0.42
1:A:353:THR:O	1:A:357:THR:OG1	2.33	0.42
1:A:412:GLU:O	1:A:413:LEU:C	2.57	0.42
1:A:352:LYS:HD3	1:A:623:MET:SD	2.60	0.42
1:A:654:THR:HG22	1:A:657:GLU:CB	2.49	0.42
1:A:903:VAL:O	1:A:907:ILE:HG13	2.19	0.42
1:A:106:VAL:O	1:A:110:ARG:CD	2.67	0.42
1:A:386:GLY:HA3	1:A:451:LYS:NZ	2.34	0.42
1:A:487:PHE:HA	1:A:493:SER:O	2.19	0.42
1:A:491:ARG:O	1:A:492:LYS:C	2.57	0.42
1:A:534:ARG:HD2	1:A:592:THR:CG2	2.49	0.42
1:A:957:PHE:N	1:A:957:PHE:CD2	2.87	0.42
1:A:179:ILE:HD13	1:A:232:ILE:HD11	2.01	0.42
1:A:549:ILE:HD11	1:A:596:VAL:HG21	2.01	0.42
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.55	0.42
1:A:459:VAL:HA	1:A:462:LEU:CD1	2.49	0.42
1:A:790:VAL:O	1:A:793:LEU:HB2	2.19	0.42
1:A:793:LEU:HA	1:A:793:LEU:HD23	1.86	0.42
1:A:512:MET:HE3	1:A:570:PRO:CB	2.49	0.42
1:A:798:VAL:O	1:A:799:THR:C	2.58	0.42
1:A:986:PHE:C	1:A:988:ALA:H	2.23	0.42
1:A:122:TYR:O	1:A:124:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LYS:NZ	1:A:749:GLU:HG2	2.34	0.42
1:A:481:LYS:CE	1:A:496:VAL:HG11	2.49	0.42
1:A:494:MET:SD	1:A:515:LYS:HE2	2.59	0.42
1:A:783:LEU:HD12	1:A:784:PRO:HD2	2.02	0.42
1:A:276:ILE:HG13	1:A:276:ILE:O	2.19	0.42
1:A:352:LYS:HB3	1:A:625:THR:HG22	2.01	0.42
1:A:760:PHE:C	1:A:760:PHE:HD1	2.21	0.42
1:A:99:ILE:HG22	1:A:103:ILE:CD1	2.40	0.42
1:A:283:VAL:O	1:A:284:HIS:C	2.57	0.42
1:A:52:LEU:O	1:A:56:GLN:HG2	2.19	0.42
1:A:683:HIS:O	1:A:684:LYS:C	2.57	0.42
1:A:776:PHE:O	1:A:777:LEU:C	2.58	0.42
1:A:106:VAL:O	1:A:110:ARG:CG	2.68	0.41
1:A:247:THR:CG2	1:A:249:LEU:HB3	2.49	0.41
1:A:282:PRO:C	1:A:284:HIS:H	2.22	0.41
1:A:247:THR:CG2	1:A:340:GLU:OE1	2.58	0.41
1:A:449:VAL:O	1:A:450:GLU:C	2.58	0.41
1:A:865:VAL:HG21	1:A:869:GLN:HB2	2.02	0.41
1:A:895:GLU:HA	1:A:898:THR:HG21	1.98	0.41
1:A:909:MET:HE1	1:A:940:SER:CB	2.49	0.41
1:A:936:SER:O	1:A:937:ILE:C	2.58	0.41
1:A:739:ASN:O	1:A:740:PHE:C	2.58	0.41
1:A:342:LEU:HD21	1:A:746:ALA:HB1	2.01	0.41
1:A:862:GLY:H	1:A:863:PRO:CD	2.29	0.41
1:A:911:ASN:HA	1:A:914:ASN:ND2	2.24	0.41
1:A:915:SER:C	1:A:917:SER:N	2.74	0.41
1:A:222:ILE:O	1:A:222:ILE:HG23	2.19	0.41
1:A:283:VAL:O	1:A:283:VAL:HG12	2.20	0.41
1:A:559:LEU:CD2	1:A:600:LEU:HB2	2.49	0.41
1:A:687:ILE:O	1:A:691:LEU:HG	2.19	0.41
1:A:126:MET:HG3	1:A:139:ARG:NH1	2.35	0.41
1:A:879:ASP:CB	1:A:882:HIS:CB	2.92	0.41
1:A:975:LEU:N	1:A:976:PRO:CD	2.84	0.41
1:A:178:SER:O	1:A:179:ILE:C	2.59	0.41
1:A:633:ILE:O	1:A:636:CYS:HB2	2.21	0.41
1:A:680:GLU:CB	1:A:681:PRO:HD2	2.28	0.41
1:A:909:MET:HB3	1:A:937:ILE:HG23	2.02	0.41
1:A:56:GLN:OE1	1:A:105:GLY:HA3	2.20	0.41
1:A:124:PRO:HB3	1:A:158:LYS:HB3	2.02	0.41
1:A:13:LEU:HD23	1:A:18:VAL:HG13	2.02	0.41
1:A:397:LYS:HB2	1:A:402:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:GLY:O	1:A:804:ALA:HB3	2.19	0.41
1:A:856:PHE:HD2	1:A:870:LEU:HD22	1.85	0.41
1:A:717:GLY:N	1:A:732:GLU:OE1	2.41	0.41
1:A:783:LEU:HD23	1:A:849:VAL:HG13	2.03	0.41
1:A:174:ARG:CB	1:A:215:ALA:HB3	2.51	0.41
1:A:256:PHE:CZ	1:A:765:ILE:HD12	2.55	0.41
1:A:898:THR:HG21	1:A:959:LEU:O	2.20	0.41
1:A:155:VAL:HG13	1:A:156:GLY:N	2.35	0.41
1:A:248:PRO:HB2	1:A:252:LYS:NZ	2.35	0.41
1:A:751:ARG:CD	1:A:817:MET:HE2	2.50	0.41
1:A:791:GLN:HB3	1:A:901:LEU:CD1	2.51	0.41
1:A:870:LEU:O	1:A:873:PHE:HB3	2.21	0.41
1:A:326:MET:HB3	1:A:331:ALA:HB3	2.03	0.41
1:A:364:CYS:O	1:A:383:SER:HA	2.21	0.41
1:A:396:LEU:CD2	1:A:401:PRO:HA	2.51	0.41
1:A:810:ASN:O	1:A:811:PRO:C	2.59	0.41
1:A:867:TYR:O	1:A:868:HIS:CB	2.69	0.41
1:A:380:ASN:ND2	1:A:382:PHE:CE2	2.79	0.41
1:A:493:SER:CB	1:A:516:GLY:HA3	2.50	0.41
1:A:754:TYR:CE2	1:A:822:ARG:NE	2.88	0.41
1:A:882:HIS:O	1:A:883:PHE:HB2	2.20	0.41
1:A:737:ASP:C	1:A:739:ASN:H	2.24	0.40
1:A:856:PHE:HE1	1:A:896:PRO:HG3	1.86	0.40
1:A:941:MET:O	1:A:942:SER:C	2.60	0.40
1:A:433:VAL:HG12	1:A:434:TYR:N	2.36	0.40
1:A:481:LYS:HE3	1:A:496:VAL:HG11	2.03	0.40
1:A:558:THR:HG22	1:A:634:ALA:CB	2.51	0.40
1:A:667:ARG:NH1	1:A:694:TYR:CE1	2.89	0.40
1:A:43:ALA:CA	1:A:120:LYS:HZ1	2.35	0.40
1:A:177:GLN:NE2	1:A:189:LYS:CE	2.84	0.40
1:A:458:GLU:HB2	1:A:461:ASN:HD22	1.87	0.40
1:A:558:THR:OG1	1:A:638:ARG:NH1	2.55	0.40
1:A:916:LEU:HD11	1:A:933:LEU:CD2	2.49	0.40
1:A:13:LEU:CD2	1:A:18:VAL:HG13	2.51	0.40
1:A:281:ASP:H	1:A:282:PRO:HD3	1.87	0.40
1:A:256:PHE:CZ	1:A:260:LEU:HD13	2.57	0.40
1:A:368:ILE:HD13	1:A:410:LEU:CG	2.52	0.40
1:A:59:ASP:O	1:A:62:VAL:HG12	2.21	0.40
1:A:834:PHE:O	1:A:838:MET:HB2	2.22	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	992/994 (100%)	789 (80%)	172 (17%)	31 (3%)	4	23

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	155	VAL
1	A	287	SER
1	A	456	ASN
1	A	458	GLU
1	A	459	VAL
1	A	677	ALA
1	A	681	PRO
1	A	227	GLY
1	A	531	GLY
1	A	795	VAL
1	A	885	GLY
1	A	406	GLN
1	A	663	LEU
1	A	863	PRO
1	A	878	GLU
1	A	900	ALA
1	A	738	ASP
1	A	889	GLU
1	A	486	GLU
1	A	840	ILE
1	A	865	VAL
1	A	453	ASN
1	A	799	THR
1	A	862	GLY
1	A	905	VAL
1	A	281	ASP
1	A	432	GLY

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Mol	Chain	Res	Type
1	A	339	VAL
1	A	539	GLY
1	A	894	PRO

### 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	840/840 (100%)	804 (96%)	36 (4%)	29	62

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	19	SER
1	A	110	ARG
1	A	180	LEU
1	A	191	THR
1	A	192	GLU
1	A	228	VAL
1	A	232	ILE
1	A	247	THR
1	A	304	VAL
1	A	353	THR
1	A	367	PHE
1	A	378	SER
1	A	379	LEU
1	A	441	THR
1	A	484	THR
1	A	519	GLU
1	A	533	THR
1	A	578	LEU
1	A	638	ARG
1	A	654	THR
1	A	681	PRO
1	A	698	THR

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Mol	Chain	Res	Type
1	A	729	THR
1	A	760	PHE
1	A	778	THR
1	A	789	PRO
1	A	791	GLN
1	A	800	ASP
1	A	805	THR
1	A	816	ILE
1	A	838	MET
1	A	867	TYR
1	A	898	THR
1	A	910	CYS
1	A	958	LYS

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

Mol	Chain	Res	Type
1	A	5	HIS
1	A	177	GLN
1	A	398	ASN
1	A	453	ASN
1	A	461	ASN
1	A	472	ASN
1	A	526	ASN
1	A	628	ASN
1	A	683	HIS
1	A	706	ASN
1	A	759	GLN
1	A	875	GLN
1	A	882	HIS
1	A	914	ASN
1	A	944	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	TG1	A	1995	-	43,48,48	1.93	13 (30%)	44,72,72	1.99	12 (27%)
3	ACP	A	1996	4	27,33,33	2.19	9 (33%)	32,52,52	1.97	8 (25%)

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	TG1	A	1995	-	-	16/33/99/99	0/3/3/3
3	ACP	A	1996	4	-	2/15/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1996	ACP	PB-O3A	7.25	1.66	1.58
2	A	1995	TG1	O4-C21	5.70	1.33	1.21
2	A	1995	TG1	C4-C5	4.34	1.37	1.34
2	A	1995	TG1	O3-C3	4.10	1.52	1.44
3	A	1996	ACP	C2-N3	3.80	1.38	1.32
3	A	1996	ACP	PB-O2B	-3.71	1.47	1.56
2	A	1995	TG1	O6-C7	3.50	1.49	1.43
2	A	1995	TG1	O1-C13	3.23	1.43	1.34
2	A	1995	TG1	C34-C11	2.88	1.57	1.53
3	A	1996	ACP	C2'-C1'	-2.76	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1995	TG1	O7-C27	2.60	1.41	1.34
2	A	1995	TG1	C21-C22	2.58	1.58	1.50
2	A	1995	TG1	C1-C2	2.48	1.58	1.54
3	A	1996	ACP	C4-N3	2.48	1.39	1.35
2	A	1995	TG1	C31-C10	2.34	1.57	1.52
3	A	1996	ACP	C2-N1	2.34	1.38	1.33
3	A	1996	ACP	O4'-C1'	2.17	1.44	1.41
2	A	1995	TG1	C1-C5	2.13	1.54	1.51
2	A	1995	TG1	O11-C11	2.10	1.46	1.42
3	A	1996	ACP	C3'-C4'	-2.09	1.47	1.53
3	A	1996	ACP	PG-O2G	-2.09	1.50	1.54
2	A	1995	TG1	C3-C4	2.07	1.53	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1995	TG1	C10-O9-C32	6.37	136.65	121.53
2	A	1995	TG1	O12-C12-C11	-4.43	123.83	128.28
3	A	1996	ACP	C5'-C4'-C3'	-4.28	99.13	115.18
3	A	1996	ACP	O5'-C5'-C4'	4.18	123.37	108.99
3	A	1996	ACP	O3G-PG-C3B	-4.04	96.60	106.40
2	A	1995	TG1	O5-C12-O12	3.45	126.19	121.62
2	A	1995	TG1	C7-C6-C5	3.42	124.16	115.41
3	A	1996	ACP	N3-C2-N1	-3.40	123.36	128.68
2	A	1995	TG1	C11-C7-C6	-3.05	97.15	103.03
2	A	1995	TG1	C24-C22-C21	3.05	132.84	120.78
3	A	1996	ACP	PA-O3A-PB	2.86	141.62	132.56
3	A	1996	ACP	C4-C5-N7	2.82	112.34	109.40
2	A	1995	TG1	C2-O1-C13	-2.78	112.89	117.53
3	A	1996	ACP	O2A-PA-O5'	2.76	120.55	107.75
3	A	1996	ACP	O2B-PB-C3B	2.68	117.52	106.58
2	A	1995	TG1	C23-C22-C21	-2.53	109.77	116.09
2	A	1995	TG1	O11-C11-C12	-2.25	98.71	106.32
2	A	1995	TG1	O7-C8-C9	2.12	110.42	106.63
2	A	1995	TG1	O7-C27-O8	2.02	128.58	123.70
2	A	1995	TG1	C3-O3-C21	2.01	121.34	117.07

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1995	TG1	O10-C32-O9-C10

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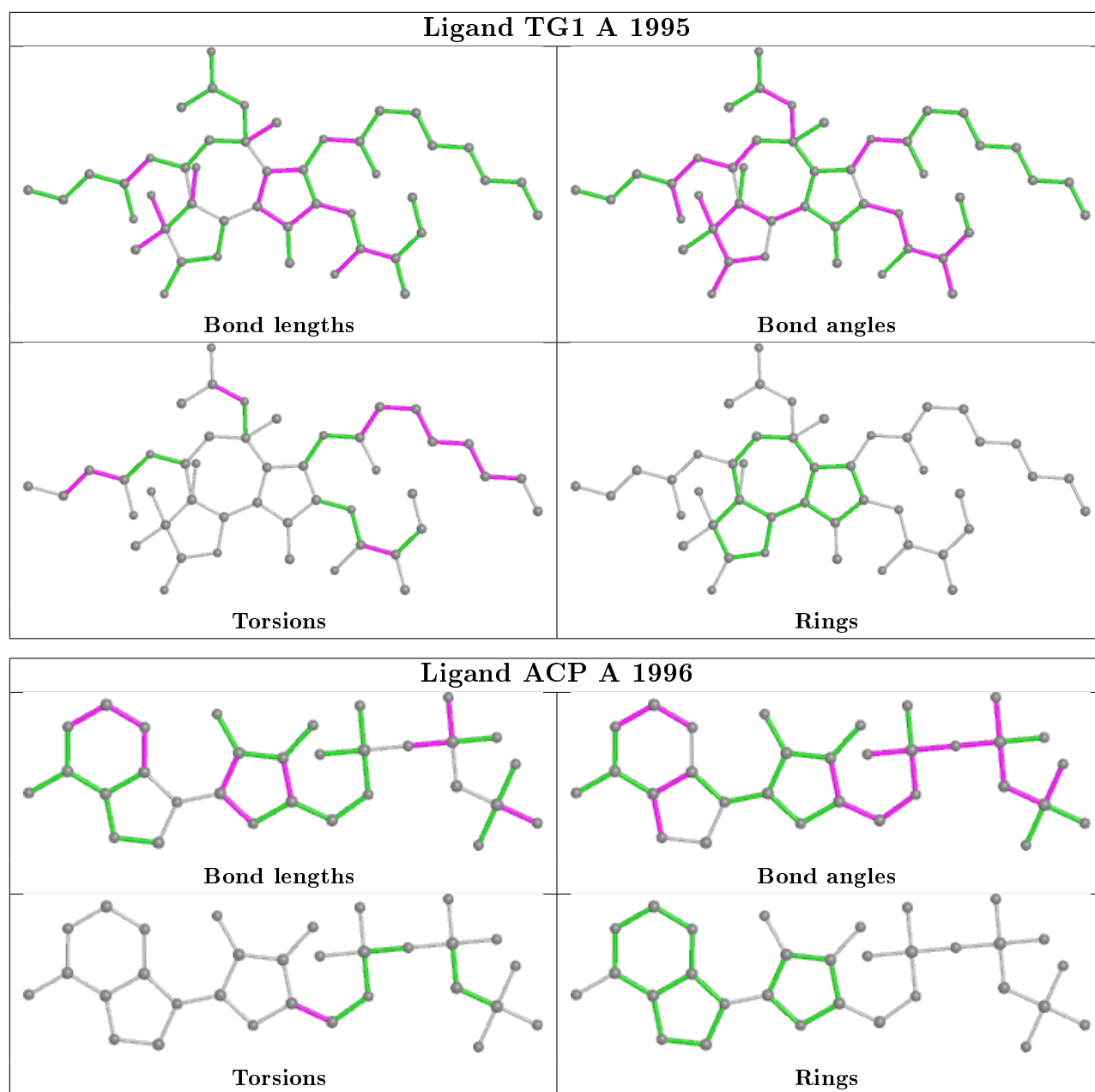
Mol	Chain	Res	Type	Atoms
2	A	1995	TG1	C33-C32-O9-C10
3	A	1996	ACP	O4'-C4'-C5'-O5'
2	A	1995	TG1	C13-C14-C15-C16
2	A	1995	TG1	O4-C21-C22-C23
2	A	1995	TG1	O4-C21-C22-C24
2	A	1995	TG1	C16-C17-C18-C19
2	A	1995	TG1	C27-C28-C29-C30
2	A	1995	TG1	C15-C16-C17-C18
2	A	1995	TG1	O3-C21-C22-C23
2	A	1995	TG1	C14-C15-C16-C17
2	A	1995	TG1	O3-C21-C22-C24
2	A	1995	TG1	C17-C18-C19-C20
3	A	1996	ACP	C3'-C4'-C5'-O5'
2	A	1995	TG1	O7-C27-C28-C29
2	A	1995	TG1	O8-C27-C28-C29
2	A	1995	TG1	O1-C13-C14-C15
2	A	1995	TG1	O2-C13-C14-C15

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1995	TG1	4	0
3	A	1996	ACP	4	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	994/994 (100%)	-0.34	29 (2%)	51 28	14, 55, 120, 168	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	505	ARG	6.1
1	A	80	GLU	5.7
1	A	286	GLY	4.8
1	A	504	SER	4.7
1	A	507	ALA	4.6
1	A	281	ASP	4.4
1	A	994	GLY	4.2
1	A	990	ASN	3.9
1	A	951	ASP	3.7
1	A	506	ALA	3.6
1	A	877	THR	3.5
1	A	280	ASN	3.2
1	A	879	ASP	3.2
1	A	82	GLU	3.2
1	A	960	LYS	3.1
1	A	964	LEU	3.1
1	A	47	LYS	3.0
1	A	78	PHE	2.9
1	A	106	VAL	2.8
1	A	878	GLU	2.7
1	A	283	VAL	2.5
1	A	50	TRP	2.5
1	A	888	CYS	2.5
1	A	508	VAL	2.4
1	A	992	LEU	2.4
1	A	503	SER	2.3
1	A	881	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	77	TRP	2.1
1	A	986	PHE	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

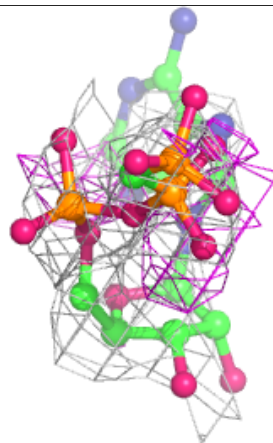
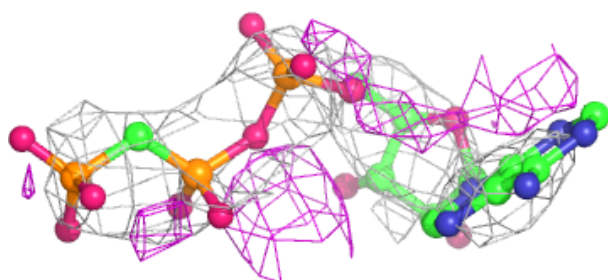
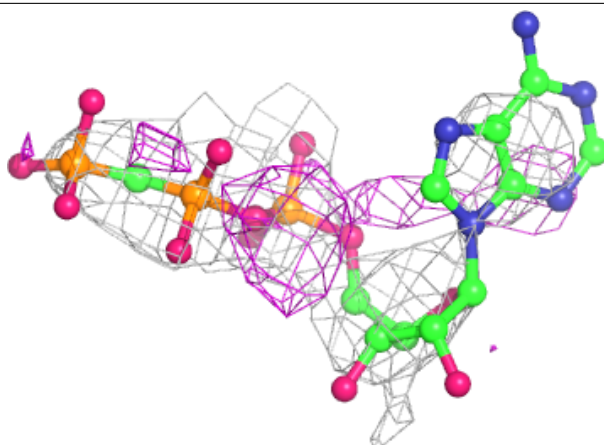
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	1997	1/1	0.47	0.43	77,77,77,77	0
3	ACP	A	1996	31/31	0.79	0.42	110,112,127,128	0
5	NA	A	1998	1/1	0.89	0.23	59,59,59,59	0
2	TG1	A	1995	46/46	0.95	0.22	52,58,69,70	0

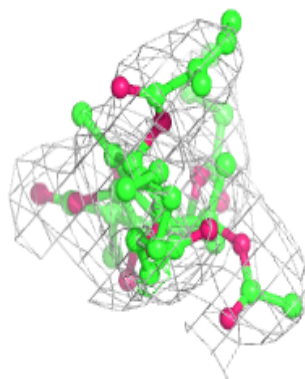
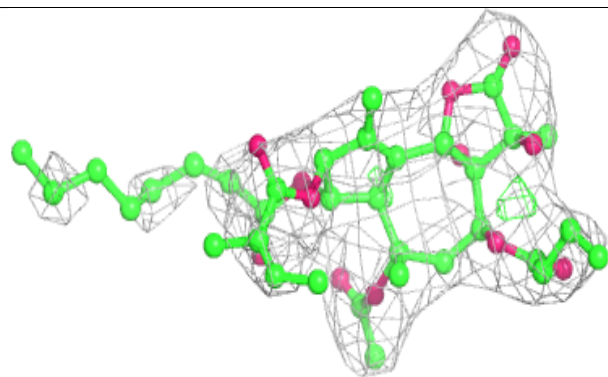
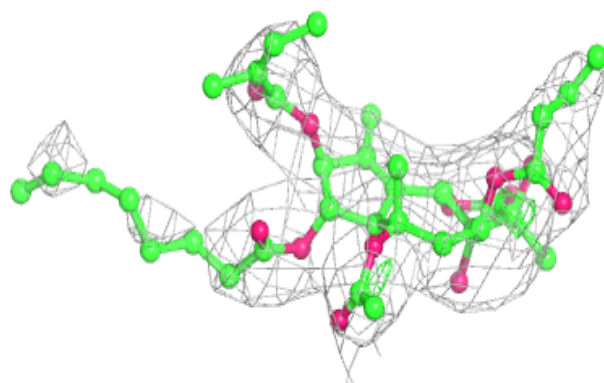
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ACP A 1996:**

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

**Electron density around TG1 A 1995:**

$2mF_o-DF_c$  (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.