



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 04:56 am GMT

PDB ID : 2C8K
Title : Crystal Structure of (SR) Calcium-ATPase E2(Tg) with partially occupied AMPPCP site
Authors : Jensen, A.M.; Sorensen, T.L.; Olesen, C.; Moller, J.V.; Nissen, P.
Deposited on : 2005-12-06
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

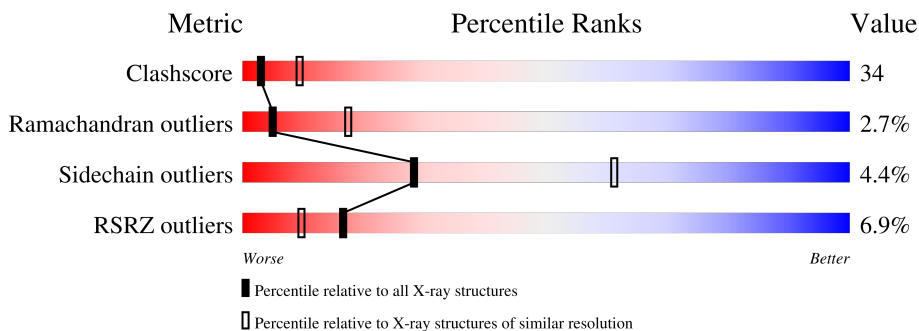
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	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	X

2 Entry composition [i](#)

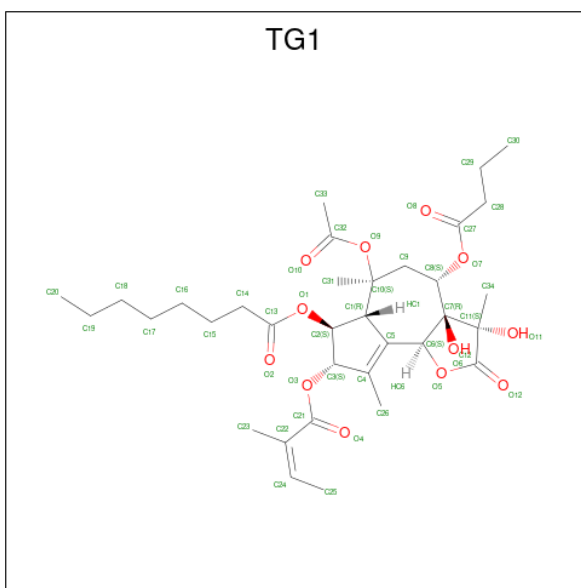
There are 5 unique types of molecules in this entry. The entry contains 7750 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

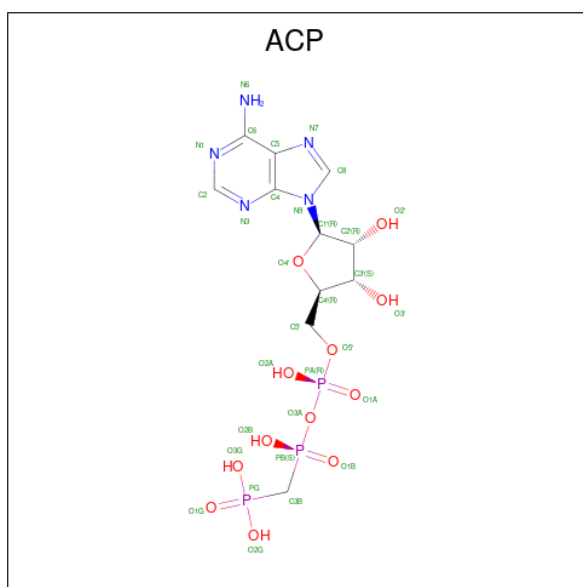
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	994	7671	4876	1287	1451	57	0	0	0

- 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: C₃₄H₅₀O₁₂).



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

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

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

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

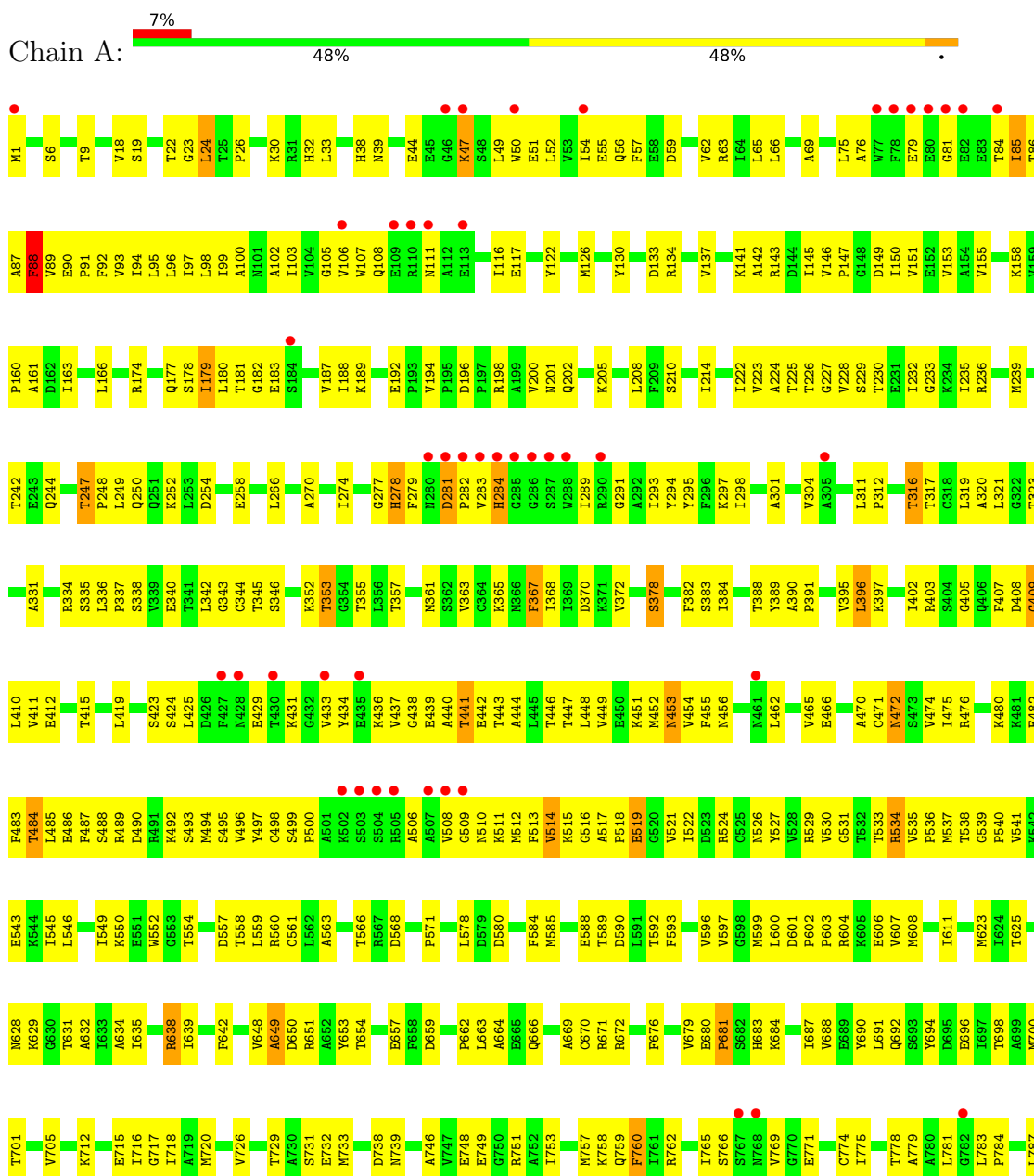
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

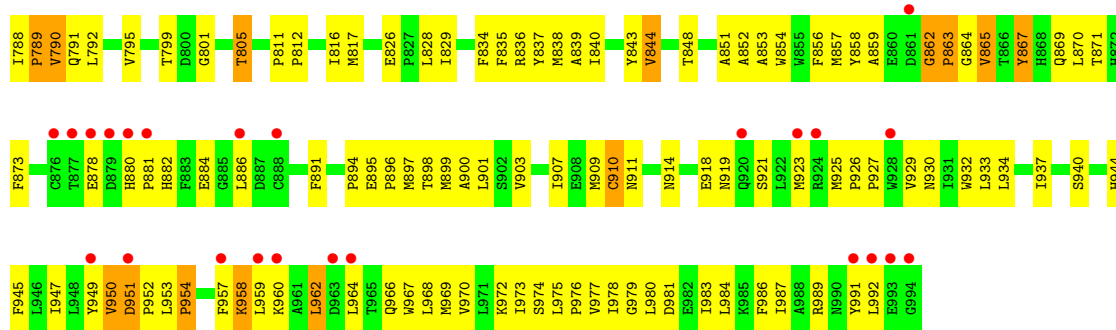
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	1	1	1	0	0

3 Residue-property plots

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

• Molecule 1: ARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.34Å 71.34Å 587.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.95 – 2.80 29.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (14.95-2.80) 92.7 (29.83-2.80)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.80Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.252 , 0.308 0.251 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtrriage
Anisotropy	0.147	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7750	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/7812	0.66	2/10592 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	GLY	N-CA-C	8.55	134.47	113.10
1	A	962	LEU	N-CA-C	-5.84	95.23	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	532	0
2	A	46	0	50	2	0
3	A	31	0	14	9	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
All	All	7750	0	7828	532	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 34.

All (532) 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:334:ARG:HH12	1:A:729:THR:HA	1.05	1.18
1:A:521:VAL:HG21	1:A:563:ALA:HB3	1.29	1.07
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.37	1.05
1:A:453:ASN:HB3	1:A:471:CYS:SG	1.97	1.04
1:A:530:VAL:HG23	1:A:533:THR:HG23	1.39	1.02
1:A:1:MET:HB2	1:A:225:THR:HG22	1.40	1.02
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.24	1.02
1:A:76:ALA:HB1	1:A:87:ALA:O	1.60	1.01
1:A:527:TYR:HB2	1:A:592:THR:HG22	1.36	1.01
1:A:247:THR:HG22	1:A:250:GLN:H	1.20	0.99
1:A:79:GLU:HG2	1:A:84:THR:HG21	1.44	0.97
1:A:342:LEU:O	1:A:345:THR:HG23	1.64	0.97
1:A:334:ARG:NH1	1:A:729:THR:HA	1.78	0.96
1:A:248:PRO:HG2	1:A:340:GLU:OE2	1.67	0.94
1:A:352:LYS:HE3	1:A:635:ILE:HD13	1.51	0.92
1:A:411:VAL:HG12	1:A:454:VAL:CG1	1.99	0.90
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.51	0.90
1:A:530:VAL:HG23	1:A:533:THR:CG2	2.02	0.89
1:A:680:GLU:H	1:A:683:HIS:HD2	1.21	0.88
1:A:560:ARG:HH21	3:A:1996:ACP:H3'	1.39	0.88
1:A:530:VAL:CG2	1:A:533:THR:HG23	2.03	0.87
1:A:192:GLU:OE1	1:A:580:ASP:HB2	1.76	0.86
1:A:950:VAL:O	1:A:954:PRO:HG2	1.77	0.85
1:A:788:ILE:HG12	1:A:897:MET:CE	2.07	0.84
1:A:865:VAL:HG11	1:A:869:GLN:HB2	1.57	0.84
1:A:161:ALA:HA	1:A:210:SER:HB2	1.60	0.84
1:A:153:VAL:HB	1:A:214:ILE:CD1	2.07	0.83
1:A:862:GLY:H	1:A:863:PRO:HD3	1.43	0.83
1:A:654:THR:HG22	1:A:657:GLU:HG3	1.62	0.81
1:A:411:VAL:HG12	1:A:454:VAL:HG11	1.63	0.81
1:A:795:VAL:HA	1:A:799:THR:OG1	1.81	0.81
1:A:680:GLU:N	1:A:683:HIS:HD2	1.78	0.81
1:A:436:LYS:HG3	1:A:443:THR:HG21	1.61	0.81
1:A:788:ILE:HG12	1:A:897:MET:HE3	1.61	0.81
1:A:549:ILE:HD11	1:A:596:VAL:HG11	1.63	0.81
1:A:521:VAL:CG2	1:A:563:ALA:HB3	2.10	0.80
1:A:1:MET:CE	1:A:229:SER:HB3	2.12	0.80
1:A:700:MET:HE3	1:A:701:THR:H	1.45	0.80
1:A:352:LYS:HB2	1:A:625:THR:HG22	1.64	0.79
1:A:788:ILE:HG22	1:A:790:VAL:HG23	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:THR:HB	1:A:496:VAL:HG12	1.64	0.78
1:A:945:PHE:HD1	1:A:949:TYR:HE2	1.28	0.78
1:A:180:LEU:HA	1:A:705:VAL:HG12	1.63	0.78
1:A:680:GLU:H	1:A:683:HIS:CD2	2.02	0.78
1:A:909:MET:CE	1:A:937:ILE:HA	2.13	0.77
1:A:177:GLN:HE22	1:A:189:LYS:NZ	1.80	0.77
1:A:436:LYS:CG	1:A:443:THR:HG21	2.14	0.77
1:A:865:VAL:HG11	1:A:869:GLN:CB	2.14	0.77
1:A:397:LYS:HB3	1:A:402:ILE:HD11	1.67	0.76
1:A:312:PRO:O	1:A:316:THR:HG23	1.85	0.76
1:A:59:ASP:HB3	1:A:62:VAL:HG12	1.68	0.76
1:A:449:VAL:HG11	1:A:472:ASN:ND2	2.01	0.76
1:A:748:GLU:HG3	1:A:817:MET:HE3	1.68	0.75
1:A:909:MET:HE3	1:A:937:ILE:HA	1.68	0.75
1:A:958:LYS:HD2	1:A:958:LYS:N	2.01	0.75
1:A:606:GLU:H	1:A:606:GLU:CD	1.87	0.75
1:A:751:ARG:HD2	1:A:817:MET:CE	2.17	0.75
1:A:958:LYS:HD2	1:A:958:LYS:H	1.52	0.75
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.69	0.75
1:A:835:PHE:O	1:A:838:MET:HB3	1.86	0.75
1:A:447:THR:HG22	1:A:451:LYS:HE2	1.69	0.74
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.27	0.74
1:A:281:ASP:OD1	1:A:282:PRO:HD3	1.87	0.74
1:A:89:VAL:O	1:A:93:VAL:HG23	1.88	0.73
1:A:471:CYS:O	1:A:474:VAL:HG22	1.87	0.73
1:A:352:LYS:CB	1:A:625:THR:HG22	2.18	0.73
1:A:748:GLU:HA	1:A:817:MET:CE	2.18	0.72
1:A:560:ARG:NH2	3:A:1996:ACP:H8	2.04	0.72
1:A:654:THR:HG22	1:A:657:GLU:CG	2.20	0.72
1:A:334:ARG:HH12	1:A:729:THR:CA	1.96	0.71
1:A:153:VAL:HB	1:A:214:ILE:HD11	1.71	0.71
1:A:788:ILE:HG23	1:A:789:PRO:HD2	1.72	0.70
1:A:382:PHE:CE2	1:A:410:LEU:HD11	2.26	0.70
1:A:247:THR:CG2	1:A:250:GLN:HG3	2.21	0.70
1:A:252:LYS:HE2	1:A:826:GLU:O	1.91	0.70
1:A:439:GLU:O	1:A:443:THR:HG22	1.91	0.70
1:A:1:MET:HE3	1:A:229:SER:HB3	1.73	0.70
1:A:651:ARG:HG2	1:A:651:ARG:HH11	1.57	0.70
1:A:62:VAL:HG23	1:A:98:LEU:HD22	1.74	0.69
1:A:19:SER:OG	1:A:22:THR:HB	1.92	0.69
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:ARG:NH2	3:A:1996:ACP:H3'	2.07	0.69
1:A:791:GLN:HB3	1:A:901:LEU:CD1	2.23	0.69
1:A:100:ALA:HA	1:A:103:ILE:HD12	1.75	0.69
1:A:298:ILE:CD1	1:A:779:ALA:HB2	2.24	0.68
1:A:453:ASN:CB	1:A:471:CYS:SG	2.77	0.68
1:A:122:TYR:HE2	1:A:726:VAL:HG21	1.59	0.68
1:A:334:ARG:O	1:A:335:SER:HB3	1.94	0.68
1:A:363:VAL:HG13	1:A:597:VAL:HG13	1.75	0.68
1:A:1:MET:O	1:A:1:MET:HG3	1.93	0.68
1:A:388:THR:HG22	1:A:389:TYR:N	2.10	0.67
1:A:515:LYS:HE3	3:A:1996:ACP:N1	2.09	0.67
1:A:99:ILE:O	1:A:103:ILE:HG13	1.94	0.67
1:A:87:ALA:O	1:A:88:PHE:HD1	1.78	0.67
1:A:431:LYS:O	1:A:433:VAL:HG23	1.95	0.67
1:A:680:GLU:CB	1:A:681:PRO:HD2	2.15	0.66
1:A:979:GLY:O	1:A:983:ILE:HG13	1.96	0.65
1:A:133:ASP:O	1:A:134:ARG:HG3	1.96	0.65
1:A:146:VAL:HG13	1:A:147:PRO:HD2	1.77	0.65
1:A:247:THR:HG23	1:A:249:LEU:H	1.61	0.65
1:A:775:ILE:O	1:A:778:THR:HG22	1.96	0.65
1:A:368:ILE:HD13	1:A:410:LEU:HD23	1.79	0.65
1:A:508:VAL:HG11	1:A:511:LYS:NZ	2.11	0.65
1:A:951:ASP:C	1:A:954:PRO:HD2	2.16	0.65
1:A:247:THR:HG22	1:A:250:GLN:HG3	1.78	0.65
1:A:122:TYR:O	1:A:158:LYS:HD3	1.97	0.64
1:A:788:ILE:CG2	1:A:790:VAL:HG23	2.27	0.64
1:A:521:VAL:HG21	1:A:563:ALA:CB	2.18	0.64
1:A:927:PRO:HB2	1:A:934:LEU:HD21	1.79	0.64
1:A:545:ILE:O	1:A:549:ILE:HG12	1.98	0.64
1:A:944:HIS:O	1:A:947:ILE:HG12	1.96	0.64
1:A:950:VAL:CG1	1:A:951:ASP:N	2.61	0.64
1:A:79:GLU:CG	1:A:84:THR:HG21	2.24	0.63
1:A:748:GLU:HA	1:A:817:MET:HE3	1.80	0.63
1:A:448:LEU:O	1:A:452:MET:HG2	1.99	0.63
1:A:472:ASN:O	1:A:476:ARG:HG3	1.98	0.63
1:A:317:THR:O	1:A:321:LEU:HG	1.97	0.63
1:A:177:GLN:NE2	1:A:189:LYS:NZ	2.46	0.63
1:A:900:ALA:O	1:A:903:VAL:HG12	1.98	0.63
1:A:751:ARG:HD2	1:A:817:MET:HE2	1.81	0.63
1:A:295:TYR:O	1:A:298:ILE:HG22	1.98	0.62
1:A:958:LYS:N	1:A:958:LYS:CD	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:CG1	1:A:454:VAL:HG11	2.30	0.62
1:A:508:VAL:HG11	1:A:511:LYS:HZ1	1.65	0.62
1:A:402:ILE:HG22	1:A:403:ARG:N	2.13	0.62
1:A:748:GLU:HA	1:A:817:MET:HE1	1.81	0.62
1:A:75:LEU:HD13	1:A:297:LYS:HB3	1.82	0.61
1:A:247:THR:HG22	1:A:250:GLN:N	2.04	0.61
1:A:500:PRO:HG3	1:A:506:ALA:HA	1.81	0.61
1:A:757:MET:HA	1:A:760:PHE:CE2	2.35	0.61
1:A:183:GLU:O	1:A:183:GLU:HG3	2.00	0.61
1:A:751:ARG:HD2	1:A:817:MET:HE1	1.83	0.61
1:A:559:LEU:HD23	1:A:600:LEU:HB2	1.83	0.61
1:A:909:MET:HE3	1:A:937:ILE:HG12	1.82	0.61
1:A:161:ALA:CA	1:A:210:SER:HB2	2.29	0.61
1:A:412:GLU:CD	1:A:529:ARG:HE	2.04	0.61
1:A:84:THR:O	1:A:86:THR:N	2.34	0.60
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.36	0.60
1:A:526:ASN:ND2	1:A:590:ASP:HA	2.16	0.60
1:A:91:PRO:O	1:A:95:LEU:HG	2.01	0.60
1:A:870:LEU:HD12	1:A:873:PHE:HB3	1.83	0.60
1:A:247:THR:HG23	1:A:340:GLU:OE1	2.01	0.60
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.83	0.60
1:A:541:VAL:O	1:A:545:ILE:HG13	2.02	0.60
1:A:903:VAL:O	1:A:907:ILE:HG13	2.02	0.60
1:A:470:ALA:O	1:A:474:VAL:HG13	2.02	0.60
1:A:859:ALA:O	1:A:863:PRO:HG3	2.02	0.60
1:A:865:VAL:HG11	1:A:869:GLN:CG	2.32	0.59
1:A:177:GLN:HE22	1:A:189:LYS:HZ3	1.49	0.59
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.01	0.59
1:A:361:MET:HB3	1:A:599:MET:HE3	1.84	0.59
1:A:700:MET:HE3	1:A:701:THR:N	2.16	0.59
1:A:298:ILE:HD13	1:A:779:ALA:HB2	1.85	0.59
1:A:527:TYR:O	1:A:592:THR:HA	2.02	0.59
1:A:550:LYS:O	1:A:554:THR:HB	2.03	0.59
1:A:411:VAL:O	1:A:415:THR:HG23	2.02	0.59
1:A:749:GLU:O	1:A:753:ILE:HG12	2.02	0.59
1:A:895:GLU:OE2	1:A:959:LEU:HD11	2.01	0.59
1:A:951:ASP:H	1:A:952:PRO:HD2	1.68	0.59
1:A:688:VAL:O	1:A:692:GLN:HG3	2.01	0.59
1:A:720:MET:HB3	1:A:738:ASP:OD1	2.03	0.58
1:A:895:GLU:CD	1:A:959:LEU:HD11	2.23	0.58
1:A:441:THR:HA	1:A:599:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:PRO:HD2	1:A:434:TYR:CE2	2.39	0.58
1:A:483:PHE:HE1	1:A:485:LEU:HD21	1.68	0.58
1:A:95:LEU:O	1:A:99:ILE:HG12	2.04	0.58
1:A:865:VAL:HG11	1:A:869:GLN:HG2	1.84	0.58
1:A:59:ASP:HB3	1:A:62:VAL:CG1	2.32	0.58
1:A:389:TYR:HB3	1:A:425:LEU:HD21	1.85	0.58
1:A:974:SER:O	1:A:977:VAL:HG23	2.03	0.58
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.39	0.58
1:A:277:GLY:C	1:A:279:PHE:H	2.07	0.58
1:A:518:PRO:HD3	1:A:561:CYS:O	2.04	0.58
1:A:654:THR:CG2	1:A:657:GLU:HG3	2.33	0.58
1:A:759:GLN:HE22	1:A:762:ARG:HH11	1.52	0.57
1:A:911:ASN:HA	1:A:914:ASN:ND2	2.06	0.57
1:A:717:GLY:N	1:A:732:GLU:OE1	2.38	0.57
1:A:331:ALA:HB1	1:A:733:MET:CE	2.34	0.57
1:A:26:PRO:O	1:A:30:LYS:HG3	2.03	0.57
1:A:436:LYS:HG3	1:A:443:THR:CG2	2.31	0.57
1:A:851:ALA:O	1:A:854:TRP:HB3	2.05	0.57
1:A:75:LEU:HD22	1:A:293:ILE:HG13	1.86	0.57
1:A:298:ILE:HD11	1:A:779:ALA:HB2	1.87	0.57
1:A:146:VAL:HG13	1:A:147:PRO:CD	2.34	0.57
1:A:177:GLN:HE22	1:A:189:LYS:HZ1	1.50	0.56
1:A:248:PRO:O	1:A:252:LYS:HG3	2.05	0.56
1:A:408:ASP:O	1:A:411:VAL:HG22	2.05	0.56
1:A:278:HIS:HA	1:A:282:PRO:HG2	1.88	0.56
1:A:352:LYS:CE	1:A:635:ILE:HD13	2.29	0.56
1:A:388:THR:HG22	1:A:390:ALA:H	1.69	0.56
1:A:895:GLU:N	1:A:896:PRO:HD2	2.19	0.56
1:A:519:GLU:OE1	1:A:519:GLU:N	2.27	0.56
1:A:950:VAL:HG12	1:A:951:ASP:N	2.20	0.56
1:A:47:LYS:HB3	1:A:51:GLU:OE1	2.06	0.56
1:A:517:ALA:HB2	3:A:1996:ACP:H4'	1.87	0.56
1:A:607:VAL:O	1:A:611:ILE:HG12	2.05	0.56
1:A:895:GLU:O	1:A:899:MET:HG2	2.06	0.56
1:A:244:GLN:CD	1:A:244:GLN:H	2.09	0.55
1:A:452:MET:O	1:A:454:VAL:N	2.39	0.55
1:A:969:MET:O	1:A:973:ILE:HG13	2.06	0.55
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.87	0.55
1:A:411:VAL:HG12	1:A:454:VAL:HG13	1.88	0.55
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.86	0.55
1:A:526:ASN:HD22	1:A:590:ASP:HA	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:ILE:HG23	1:A:977:VAL:HG21	1.87	0.55
1:A:411:VAL:CB	1:A:454:VAL:HG11	2.36	0.55
1:A:557:ASP:HB3	1:A:559:LEU:HG	1.89	0.55
1:A:659:ASP:OD1	1:A:683:HIS:HE1	1.89	0.55
1:A:691:LEU:O	1:A:696:GLU:HB2	2.07	0.55
1:A:412:GLU:OE1	1:A:529:ARG:NE	2.38	0.55
1:A:483:PHE:CE1	1:A:578:LEU:HD22	2.42	0.55
1:A:122:TYR:HE2	1:A:726:VAL:CG2	2.19	0.55
1:A:530:VAL:HG23	1:A:530:VAL:O	2.07	0.55
1:A:910:CYS:SG	1:A:978:ILE:HD11	2.47	0.55
1:A:32:HIS:HB3	1:A:146:VAL:CG1	2.37	0.54
1:A:603:PRO:HG2	1:A:638:ARG:HD3	1.88	0.54
1:A:651:ARG:HG2	1:A:651:ARG:NH1	2.22	0.54
1:A:361:MET:HE3	1:A:599:MET:HG3	1.87	0.54
1:A:465:VAL:O	1:A:465:VAL:HG12	2.07	0.54
1:A:92:PHE:CE2	1:A:96:LEU:HD11	2.41	0.54
1:A:367:PHE:CD1	1:A:367:PHE:C	2.81	0.54
1:A:840:ILE:O	1:A:844:VAL:HG13	2.07	0.54
1:A:32:HIS:CB	1:A:146:VAL:HG11	2.37	0.54
1:A:784:PRO:HG3	1:A:873:PHE:CD2	2.42	0.54
1:A:196:ASP:OD1	1:A:198:ARG:N	2.36	0.54
1:A:654:THR:CG2	1:A:657:GLU:H	2.20	0.54
1:A:278:HIS:HA	1:A:282:PRO:CG	2.38	0.54
1:A:608:MET:SD	1:A:639:ILE:HA	2.48	0.54
1:A:353:THR:HA	1:A:357:THR:OG1	2.07	0.54
1:A:962:LEU:O	1:A:966:GLN:HB2	2.08	0.54
1:A:515:LYS:HE3	3:A:1996:ACP:C6	2.38	0.54
1:A:436:LYS:CD	1:A:443:THR:HG21	2.38	0.54
1:A:535:VAL:HG13	1:A:536:PRO:HD2	1.90	0.54
1:A:894:PRO:O	1:A:898:THR:HG23	2.08	0.54
1:A:853:ALA:O	1:A:856:PHE:HB2	2.07	0.53
1:A:909:MET:CE	1:A:940:SER:HB2	2.38	0.53
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.90	0.53
1:A:235:ILE:HD13	1:A:705:VAL:HG22	1.89	0.53
1:A:239:MET:O	1:A:242:THR:HG22	2.09	0.53
1:A:363:VAL:CG1	1:A:597:VAL:HG13	2.38	0.53
1:A:402:ILE:CG2	1:A:403:ARG:N	2.72	0.53
1:A:986:PHE:CE1	1:A:989:ARG:HD2	2.43	0.53
1:A:593:PHE:CZ	1:A:596:VAL:HG12	2.44	0.53
1:A:23:GLY:HA3	1:A:130:TYR:O	2.09	0.53
1:A:76:ALA:HB1	1:A:88:PHE:HD1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:O	1:A:258:GLU:HG2	2.09	0.53
1:A:455:PHE:O	1:A:456:ASN:HB2	2.09	0.53
1:A:281:ASP:CG	1:A:282:PRO:HD3	2.28	0.53
1:A:527:TYR:CE2	1:A:534:ARG:NH2	2.77	0.53
1:A:676:PHE:CE2	1:A:687:ILE:HD13	2.43	0.53
1:A:791:GLN:HB3	1:A:901:LEU:HD12	1.91	0.53
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.91	0.52
1:A:489:ARG:O	1:A:492:LYS:HE3	2.10	0.52
1:A:235:ILE:HG21	1:A:705:VAL:HG22	1.91	0.52
1:A:200:VAL:HG12	1:A:681:PRO:HG3	1.92	0.52
1:A:894:PRO:CB	1:A:958:LYS:HG3	2.39	0.52
1:A:962:LEU:N	1:A:966:GLN:OE1	2.41	0.52
1:A:59:ASP:O	1:A:62:VAL:HG12	2.10	0.52
1:A:486:GLU:OE2	1:A:584:PHE:HE2	1.91	0.52
1:A:865:VAL:HG12	1:A:867:TYR:H	1.73	0.52
1:A:76:ALA:CB	1:A:87:ALA:O	2.48	0.52
1:A:57:PHE:HE1	1:A:102:ALA:HB2	1.74	0.52
1:A:748:GLU:CG	1:A:817:MET:HE3	2.39	0.52
1:A:49:LEU:HD23	1:A:52:LEU:HD12	1.92	0.52
1:A:462:LEU:HB3	1:A:466:GLU:CD	2.29	0.52
1:A:178:SER:O	1:A:180:LEU:N	2.42	0.52
1:A:388:THR:CG2	1:A:389:TYR:N	2.73	0.51
1:A:446:THR:HB	1:A:472:ASN:OD1	2.10	0.51
1:A:538:THR:OG1	1:A:541:VAL:HG23	2.10	0.51
1:A:865:VAL:CG1	1:A:869:GLN:H	2.23	0.51
1:A:898:THR:HG22	1:A:958:LYS:HB2	1.91	0.51
1:A:304:VAL:HG21	1:A:789:PRO:HA	1.91	0.51
1:A:844:VAL:O	1:A:848:THR:HG23	2.11	0.51
1:A:284:HIS:O	1:A:284:HIS:ND1	2.43	0.51
1:A:829:ILE:HG21	2:A:1995:TG1:H333	1.91	0.51
1:A:945:PHE:HD1	1:A:949:TYR:CE2	2.17	0.51
1:A:480:LYS:O	1:A:498:CYS:HA	2.11	0.51
1:A:623:MET:HG2	1:A:625:THR:HG23	1.93	0.51
1:A:950:VAL:HG13	1:A:952:PRO:HD2	1.92	0.51
1:A:99:ILE:HG22	1:A:103:ILE:HD11	1.92	0.50
1:A:517:ALA:O	1:A:521:VAL:HG22	2.11	0.50
1:A:153:VAL:CB	1:A:214:ILE:HD11	2.40	0.50
1:A:662:PRO:O	1:A:664:ALA:N	2.44	0.50
1:A:107:TRP:CD1	1:A:111:ASN:ND2	2.80	0.50
1:A:301:ALA:HA	1:A:789:PRO:HG3	1.92	0.50
1:A:629:LYS:O	1:A:632:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:LEU:O	1:A:968:LEU:HD12	2.11	0.50
1:A:244:GLN:CD	1:A:244:GLN:N	2.65	0.50
1:A:126:MET:SD	1:A:141:LYS:HG2	2.52	0.50
1:A:277:GLY:O	1:A:279:PHE:N	2.45	0.50
1:A:474:VAL:HG23	1:A:475:ILE:N	2.26	0.50
1:A:519:GLU:H	1:A:519:GLU:CD	2.04	0.50
1:A:50:TRP:NE1	1:A:54:ILE:HD11	2.27	0.50
1:A:18:VAL:HG22	1:A:19:SER:N	2.26	0.50
1:A:352:LYS:HD2	1:A:625:THR:CG2	2.42	0.49
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.77	0.49
1:A:650:ASP:OD2	1:A:672:ARG:HD3	2.12	0.49
1:A:765:ILE:O	1:A:769:VAL:HG23	2.11	0.49
1:A:967:TRP:O	1:A:970:VAL:HB	2.12	0.49
1:A:783:LEU:HD12	1:A:784:PRO:HD2	1.94	0.49
1:A:856:PHE:O	1:A:864:GLY:N	2.45	0.49
1:A:51:GLU:O	1:A:55:GLU:HG3	2.12	0.49
1:A:32:HIS:HB3	1:A:146:VAL:HG11	1.95	0.49
1:A:415:THR:HA	1:A:475:ILE:HG21	1.95	0.49
1:A:150:ILE:HD12	1:A:150:ILE:N	2.28	0.49
1:A:361:MET:HB3	1:A:599:MET:CE	2.43	0.49
1:A:408:ASP:HB2	1:A:531:GLY:HA2	1.95	0.49
1:A:512:MET:HE1	1:A:571:PRO:HD2	1.93	0.49
1:A:331:ALA:HB1	1:A:733:MET:HE1	1.94	0.49
1:A:604:ARG:HH11	1:A:739:ASN:ND2	2.11	0.49
1:A:671:ARG:HB3	1:A:694:TYR:CE2	2.48	0.49
1:A:901:LEU:C	1:A:901:LEU:HD23	2.32	0.49
1:A:150:ILE:N	1:A:150:ILE:CD1	2.76	0.48
1:A:319:LEU:HG	1:A:757:MET:HE1	1.94	0.48
1:A:852:ALA:HB2	1:A:900:ALA:HB2	1.94	0.48
1:A:909:MET:HE1	1:A:940:SER:HB2	1.95	0.48
1:A:926:PRO:HG2	1:A:929:VAL:HG23	1.95	0.48
1:A:516:GLY:HA2	3:A:1996:ACP:N3	2.28	0.48
1:A:79:GLU:HG2	1:A:84:THR:CG2	2.31	0.48
1:A:788:ILE:HG12	1:A:897:MET:HE1	1.94	0.48
1:A:151:VAL:CG2	1:A:223:VAL:HG23	2.43	0.48
1:A:227:GLY:O	1:A:230:THR:HG22	2.13	0.48
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.48	0.48
1:A:900:ALA:C	1:A:903:VAL:HG12	2.34	0.48
1:A:670:CYS:HG	1:A:690:TYR:HD2	1.62	0.48
1:A:950:VAL:O	1:A:954:PRO:CG	2.57	0.48
1:A:352:LYS:HD2	1:A:625:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LYS:HB3	1:A:402:ILE:CD1	2.41	0.48
1:A:897:MET:SD	1:A:958:LYS:HE2	2.54	0.48
1:A:950:VAL:CG1	1:A:951:ASP:H	2.27	0.48
1:A:415:THR:HA	1:A:475:ILE:HD13	1.95	0.48
1:A:857:MET:O	1:A:858:TYR:HB2	2.14	0.48
1:A:968:LEU:O	1:A:972:LYS:HG2	2.14	0.48
1:A:715:GLU:C	1:A:716:ILE:HD12	2.35	0.47
1:A:781:LEU:O	1:A:871:THR:HG23	2.14	0.47
1:A:894:PRO:HB2	1:A:958:LYS:HB3	1.95	0.47
1:A:85:ILE:HG23	1:A:86:THR:N	2.28	0.47
1:A:291:GLY:O	1:A:294:TYR:HB3	2.14	0.47
1:A:758:LYS:HG3	1:A:828:LEU:HD22	1.95	0.47
1:A:918:GLU:HG2	1:A:919:ASN:OD1	2.13	0.47
1:A:945:PHE:CD1	1:A:949:TYR:HE2	2.19	0.47
1:A:865:VAL:HG21	1:A:869:GLN:HB2	1.96	0.47
1:A:230:THR:HG23	1:A:233:GLY:H	1.78	0.47
1:A:771:GLU:O	1:A:774:CYS:HB3	2.14	0.47
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.49	0.47
1:A:153:VAL:HB	1:A:214:ILE:HD12	1.93	0.47
1:A:355:THR:HG21	1:A:720:MET:CE	2.45	0.47
1:A:512:MET:O	1:A:566:THR:HA	2.15	0.47
1:A:527:TYR:HB2	1:A:592:THR:CG2	2.26	0.47
1:A:898:THR:CG2	1:A:958:LYS:HB2	2.44	0.47
1:A:1:MET:SD	1:A:229:SER:HB3	2.55	0.47
1:A:527:TYR:CB	1:A:592:THR:HG22	2.26	0.47
1:A:69:ALA:HB2	1:A:94:ILE:HG21	1.97	0.47
1:A:94:ILE:O	1:A:97:ILE:HB	2.15	0.47
1:A:482:GLU:HG3	1:A:497:TYR:HD2	1.80	0.47
1:A:648:VAL:O	1:A:649:ALA:C	2.52	0.47
1:A:687:ILE:O	1:A:691:LEU:HG	2.14	0.47
1:A:921:SER:OG	1:A:923:MET:HG2	2.15	0.47
1:A:192:GLU:CD	1:A:580:ASP:HB2	2.34	0.46
1:A:361:MET:SD	1:A:601:ASP:HB2	2.55	0.46
1:A:766:SER:O	1:A:769:VAL:HB	2.16	0.46
1:A:593:PHE:HZ	1:A:596:VAL:HG12	1.79	0.46
1:A:880:HIS:N	1:A:881:PRO:HD2	2.30	0.46
1:A:896:PRO:O	1:A:899:MET:HB2	2.16	0.46
1:A:495:SER:HB3	1:A:514:VAL:HB	1.98	0.46
1:A:518:PRO:HA	1:A:563:ALA:HB2	1.97	0.46
1:A:950:VAL:HG13	1:A:951:ASP:H	1.80	0.46
1:A:487:PHE:HA	1:A:493:SER:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:THR:HG22	1:A:389:TYR:H	1.80	0.46
1:A:388:THR:C	1:A:390:ALA:H	2.19	0.46
1:A:429:GLU:N	1:A:429:GLU:CD	2.69	0.46
1:A:628:ASN:OD1	1:A:631:THR:HB	2.16	0.46
1:A:969:MET:O	1:A:969:MET:HE3	2.16	0.46
1:A:895:GLU:HG3	1:A:959:LEU:HD11	1.96	0.46
1:A:405:GLY:C	1:A:407:PHE:H	2.19	0.46
1:A:788:ILE:HG22	1:A:790:VAL:H	1.80	0.46
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.46	0.46
1:A:174:ARG:NE	1:A:188:ILE:HG12	2.31	0.46
1:A:181:THR:OG1	1:A:183:GLU:HG2	2.15	0.46
1:A:909:MET:HE3	1:A:937:ILE:CA	2.43	0.46
1:A:949:TYR:C	1:A:950:VAL:O	2.53	0.46
1:A:480:LYS:N	1:A:499:SER:O	2.35	0.45
1:A:546:LEU:O	1:A:549:ILE:HB	2.15	0.45
1:A:44:GLU:OE2	1:A:117:GLU:HB2	2.16	0.45
1:A:760:PHE:CD1	1:A:760:PHE:C	2.90	0.45
1:A:39:ASN:CG	1:A:226:THR:OG1	2.54	0.45
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.83	0.45
1:A:177:GLN:NE2	1:A:189:LYS:HZ3	2.13	0.45
1:A:372:VAL:HG13	1:A:541:VAL:HG22	1.97	0.45
1:A:408:ASP:O	1:A:409:GLY:C	2.54	0.45
1:A:596:VAL:HG23	1:A:597:VAL:N	2.30	0.45
1:A:953:LEU:N	1:A:954:PRO:CD	2.79	0.45
1:A:558:THR:HG22	1:A:634:ALA:HB1	1.97	0.45
1:A:666:GLN:HG2	1:A:690:TYR:CE2	2.52	0.45
1:A:331:ALA:HB1	1:A:733:MET:HE2	1.98	0.45
1:A:388:THR:HG22	1:A:390:ALA:N	2.32	0.45
1:A:733:MET:HE1	1:A:746:ALA:CB	2.46	0.45
1:A:33:LEU:HD11	1:A:38:HIS:ND1	2.32	0.45
1:A:498:CYS:O	1:A:510:ASN:HA	2.16	0.45
1:A:684:LYS:O	1:A:688:VAL:HG23	2.17	0.45
1:A:222:ILE:HG23	1:A:222:ILE:O	2.16	0.45
1:A:270:ALA:O	1:A:274:ILE:HG12	2.17	0.45
1:A:408:ASP:O	1:A:410:LEU:N	2.50	0.45
1:A:446:THR:O	1:A:449:VAL:HB	2.16	0.45
1:A:834:PHE:O	1:A:838:MET:HB2	2.17	0.45
1:A:837:TYR:HB2	2:A:1995:TG1:C33	2.47	0.45
1:A:895:GLU:CG	1:A:959:LEU:HD11	2.47	0.45
1:A:568:ASP:OD2	1:A:592:THR:HG21	2.17	0.45
1:A:202:GLN:OE1	1:A:489:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:PHE:CZ	1:A:648:VAL:HG13	2.52	0.44
1:A:166:LEU:HD11	1:A:222:ILE:HB	1.99	0.44
1:A:984:LEU:HA	1:A:987:ILE:HG12	1.99	0.44
1:A:56:GLN:OE1	1:A:105:GLY:HA3	2.18	0.44
1:A:783:LEU:HD12	1:A:784:PRO:CD	2.48	0.44
1:A:50:TRP:O	1:A:54:ILE:HG13	2.18	0.44
1:A:539:GLY:N	1:A:540:PRO:HD2	2.33	0.44
1:A:811:PRO:HA	1:A:812:PRO:HD3	1.84	0.44
1:A:969:MET:HE3	1:A:972:LYS:HG3	1.99	0.44
1:A:974:SER:C	1:A:976:PRO:HD2	2.38	0.44
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.82	0.44
1:A:242:THR:HG23	1:A:712:LYS:NZ	2.33	0.44
1:A:278:HIS:HA	1:A:282:PRO:CD	2.48	0.44
1:A:395:VAL:C	1:A:396:LEU:HD23	2.38	0.44
1:A:717:GLY:O	1:A:731:SER:HB2	2.18	0.44
1:A:886:LEU:N	1:A:886:LEU:HD23	2.33	0.44
1:A:39:ASN:OD1	1:A:226:THR:OG1	2.33	0.44
1:A:383:SER:C	1:A:384:ILE:HD12	2.38	0.44
1:A:865:VAL:CG1	1:A:869:GLN:HB2	2.41	0.44
1:A:909:MET:HE3	1:A:937:ILE:HG23	2.00	0.44
1:A:482:GLU:HG3	1:A:497:TYR:CD2	2.53	0.43
1:A:559:LEU:CD2	1:A:600:LEU:HB2	2.46	0.43
1:A:628:ASN:OD1	1:A:628:ASN:O	2.36	0.43
1:A:38:HIS:CD2	1:A:143:ARG:HH22	2.36	0.43
1:A:147:PRO:HA	1:A:223:VAL:CG1	2.49	0.43
1:A:865:VAL:HG11	1:A:869:GLN:H	1.83	0.43
1:A:949:TYR:O	1:A:950:VAL:O	2.36	0.43
1:A:412:GLU:O	1:A:415:THR:N	2.52	0.43
1:A:236:ARG:O	1:A:236:ARG:HG2	2.17	0.43
1:A:411:VAL:HA	1:A:454:VAL:HG21	2.00	0.43
1:A:90:GLU:OE2	1:A:789:PRO:HB2	2.19	0.43
1:A:281:ASP:H	1:A:282:PRO:CD	2.32	0.43
1:A:423:SER:OG	1:A:442:GLU:HB2	2.19	0.43
1:A:444:ALA:O	1:A:447:THR:N	2.51	0.43
1:A:543:GLU:OE1	1:A:543:GLU:HA	2.17	0.43
1:A:790:VAL:HB	1:A:957:PHE:CE1	2.53	0.43
1:A:654:THR:HG22	1:A:657:GLU:H	1.82	0.43
1:A:784:PRO:HG3	1:A:873:PHE:CG	2.54	0.43
1:A:340:GLU:O	1:A:343:GLY:N	2.52	0.43
1:A:870:LEU:HD12	1:A:870:LEU:O	2.19	0.43
1:A:283:VAL:O	1:A:284:HIS:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:MET:O	1:A:589:THR:HG23	2.18	0.43
1:A:792:LEU:O	1:A:795:VAL:HB	2.19	0.43
1:A:980:LEU:HD12	1:A:980:LEU:O	2.19	0.43
1:A:106:VAL:HG13	1:A:107:TRP:N	2.34	0.43
1:A:407:PHE:O	1:A:411:VAL:HG13	2.19	0.43
1:A:521:VAL:CG2	1:A:563:ALA:CB	2.90	0.43
1:A:79:GLU:OE1	1:A:79:GLU:N	2.52	0.42
1:A:142:ALA:HA	1:A:145:ILE:CD1	2.49	0.42
1:A:178:SER:C	1:A:180:LEU:N	2.72	0.42
1:A:370:ASP:HB3	1:A:378:SER:O	2.19	0.42
1:A:521:VAL:HG23	1:A:522:ILE:N	2.34	0.42
1:A:783:LEU:CD1	1:A:784:PRO:HD2	2.49	0.42
1:A:546:LEU:O	1:A:549:ILE:N	2.52	0.42
1:A:933:LEU:O	1:A:937:ILE:HG13	2.19	0.42
1:A:391:PRO:HD2	1:A:434:TYR:CD2	2.54	0.42
1:A:524:ARG:HD2	1:A:588:GLU:O	2.18	0.42
1:A:966:GLN:O	1:A:970:VAL:HG23	2.20	0.42
1:A:716:ILE:HD12	1:A:716:ILE:N	2.34	0.42
1:A:791:GLN:H	1:A:791:GLN:HG3	1.62	0.42
1:A:397:LYS:CB	1:A:402:ILE:HD11	2.45	0.42
1:A:449:VAL:HG21	1:A:472:ASN:HD21	1.85	0.42
1:A:500:PRO:HG3	1:A:509:GLY:HA2	2.00	0.42
1:A:840:ILE:O	1:A:843:TYR:HB3	2.20	0.42
1:A:894:PRO:CG	1:A:959:LEU:HG	2.50	0.42
1:A:277:GLY:C	1:A:279:PHE:N	2.73	0.42
1:A:1:MET:SD	1:A:229:SER:CB	3.08	0.42
1:A:748:GLU:CA	1:A:817:MET:HE3	2.48	0.42
1:A:24:LEU:HD22	1:A:149:ASP:CB	2.44	0.42
1:A:32:HIS:HB2	1:A:146:VAL:HG11	2.00	0.42
1:A:63:ARG:O	1:A:66:LEU:N	2.53	0.42
1:A:200:VAL:O	1:A:201:ASN:C	2.58	0.42
1:A:174:ARG:HA	1:A:187:VAL:O	2.20	0.42
1:A:440:ALA:HA	1:A:443:THR:CG2	2.49	0.42
1:A:560:ARG:HH21	3:A:1996:ACP:H8	1.79	0.42
1:A:839:ALA:O	1:A:840:ILE:C	2.58	0.42
1:A:684:LYS:HD3	1:A:700:MET:CE	2.49	0.42
1:A:472:ASN:HD22	1:A:472:ASN:HA	1.75	0.41
1:A:653:TYR:O	1:A:676:PHE:HA	2.19	0.41
1:A:49:LEU:HA	1:A:52:LEU:HD12	2.02	0.41
1:A:163:ILE:HB	1:A:208:LEU:HB2	2.01	0.41
1:A:205:LYS:NZ	1:A:488:SER:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:VAL:O	1:A:283:VAL:HG23	2.20	0.41
1:A:336:LEU:N	1:A:337:PRO:CD	2.84	0.41
1:A:6:SER:HA	1:A:194:VAL:O	2.19	0.41
1:A:178:SER:O	1:A:181:THR:N	2.54	0.41
1:A:278:HIS:CA	1:A:282:PRO:HG2	2.50	0.41
1:A:372:VAL:HG11	1:A:541:VAL:HG21	2.01	0.41
1:A:424:SER:O	1:A:437:VAL:HB	2.20	0.41
1:A:801:GLY:O	1:A:805:THR:HG23	2.19	0.41
1:A:367:PHE:CE2	1:A:596:VAL:HG13	2.55	0.41
1:A:388:THR:CG2	1:A:389:TYR:H	2.34	0.41
1:A:865:VAL:C	1:A:867:TYR:H	2.22	0.41
1:A:92:PHE:O	1:A:96:LEU:HG	2.21	0.41
1:A:836:ARG:HH21	1:A:981:ASP:CG	2.24	0.41
1:A:18:VAL:CG2	1:A:19:SER:N	2.84	0.41
1:A:59:ASP:CB	1:A:62:VAL:HG12	2.45	0.41
1:A:116:ILE:HG23	1:A:236:ARG:HG3	2.03	0.41
1:A:247:THR:CG2	1:A:249:LEU:H	2.32	0.41
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.93	0.41
1:A:320:ALA:O	1:A:323:THR:HB	2.20	0.41
1:A:474:VAL:CG2	1:A:475:ILE:N	2.84	0.41
1:A:535:VAL:CG1	1:A:536:PRO:HD2	2.49	0.41
1:A:653:TYR:CE2	1:A:669:ALA:HB1	2.55	0.41
1:A:701:THR:HA	1:A:718:ILE:O	2.21	0.41
1:A:733:MET:HE1	1:A:746:ALA:HB1	2.03	0.41
1:A:601:ASP:HA	1:A:602:PRO:HD2	1.83	0.41
1:A:854:TRP:O	1:A:857:MET:O	2.38	0.41
1:A:862:GLY:H	1:A:863:PRO:CD	2.21	0.41
1:A:909:MET:HE2	1:A:940:SER:HB2	2.02	0.41
1:A:151:VAL:HG21	1:A:223:VAL:HG23	2.03	0.40
1:A:854:TRP:O	1:A:857:MET:N	2.55	0.40
1:A:930:ASN:OD1	1:A:932:TRP:HB2	2.21	0.40
1:A:873:PHE:HB2	1:A:891:PHE:CG	2.56	0.40
1:A:898:THR:CG2	1:A:958:LYS:CB	2.99	0.40
1:A:1:MET:HA	1:A:224:ALA:O	2.20	0.40
1:A:178:SER:O	1:A:182:GLY:N	2.55	0.40
1:A:411:VAL:CA	1:A:454:VAL:HG11	2.50	0.40
1:A:483:PHE:CE1	1:A:485:LEU:HD21	2.53	0.40
1:A:954:PRO:HA	1:A:958:LYS:O	2.21	0.40
1:A:352:LYS:HB3	1:A:625:THR:HG22	1.98	0.40
1:A:517:ALA:HA	3:A:1996:ACP:O2'	2.21	0.40
1:A:991:TYR:CG	1:A:992:LEU:N	2.89	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	992/994 (100%)	864 (87%)	101 (10%)	27 (3%)	5 17

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ILE
1	A	453	ASN
1	A	882	HIS
1	A	884	GLU
1	A	958	LYS
1	A	960	LYS
1	A	278	HIS
1	A	663	LEU
1	A	950	VAL
1	A	47	LYS
1	A	284	HIS
1	A	649	ALA
1	A	878	GLU
1	A	155	VAL
1	A	438	GLY
1	A	863	PRO
1	A	88	PHE
1	A	108	GLN
1	A	179	ILE
1	A	281	ASP
1	A	409	GLY
1	A	975	LEU
1	A	289	ILE
1	A	681	PRO
1	A	865	VAL

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Mol	Chain	Res	Type
1	A	862	GLY
1	A	951	ASP

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	840/840 (100%)	803 (96%)	37 (4%)	28 61

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	24	LEU
1	A	88	PHE
1	A	160	PRO
1	A	179	ILE
1	A	228	VAL
1	A	232	ILE
1	A	247	THR
1	A	316	THR
1	A	338	SER
1	A	344	CYS
1	A	346	SER
1	A	353	THR
1	A	367	PHE
1	A	378	SER
1	A	396	LEU
1	A	441	THR
1	A	472	ASN
1	A	484	THR
1	A	490	ASP
1	A	494	MET
1	A	514	VAL
1	A	519	GLU
1	A	534	ARG

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Mol	Chain	Res	Type
1	A	537	MET
1	A	638	ARG
1	A	698	THR
1	A	760	PHE
1	A	789	PRO
1	A	790	VAL
1	A	805	THR
1	A	816	ILE
1	A	844	VAL
1	A	867	TYR
1	A	910	CYS
1	A	925	MET
1	A	954	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	177	GLN
1	A	472	ASN
1	A	526	ASN
1	A	683	HIS
1	A	706	ASN
1	A	759	GLN
1	A	796	ASN
1	A	875	GLN
1	A	914	ASN
1	A	944	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

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
3	ACP	A	1996	4	27,33,33	1.94	6 (22%)	32,52,52	2.05	10 (31%)
2	TG1	A	1995	-	43,48,48	1.95	13 (30%)	44,72,72	1.94	9 (20%)

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
3	ACP	A	1996	4	-	2/15/38/38	0/3/3/3
2	TG1	A	1995	-	-	12/33/99/99	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1995	TG1	O4-C21	5.58	1.33	1.21
3	A	1996	ACP	PB-O3A	5.57	1.64	1.58
3	A	1996	ACP	PB-O2B	-4.14	1.46	1.56
2	A	1995	TG1	C4-C5	4.11	1.37	1.34
2	A	1995	TG1	O3-C3	3.92	1.52	1.44
2	A	1995	TG1	O1-C13	3.60	1.44	1.34
2	A	1995	TG1	O6-C7	3.58	1.49	1.43
2	A	1995	TG1	C34-C11	3.27	1.57	1.53
3	A	1996	ACP	C2'-C1'	-3.22	1.48	1.53
3	A	1996	ACP	C2-N3	2.94	1.36	1.32
2	A	1995	TG1	C31-C10	2.72	1.58	1.52
2	A	1995	TG1	C21-C22	2.67	1.59	1.50
2	A	1995	TG1	O7-C27	2.60	1.41	1.34
3	A	1996	ACP	PG-O2G	-2.50	1.49	1.54
2	A	1995	TG1	O11-C11	2.35	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1995	TG1	C11-C7	2.29	1.58	1.55
3	A	1996	ACP	C3'-C4'	-2.24	1.47	1.53
2	A	1995	TG1	C1-C2	2.11	1.58	1.54
2	A	1995	TG1	C9-C10	2.07	1.57	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1995	TG1	C10-O9-C32	6.44	136.82	121.53
3	A	1996	ACP	O5'-C5'-C4'	4.54	124.63	108.99
3	A	1996	ACP	C5'-C4'-C3'	-4.15	99.62	115.18
3	A	1996	ACP	O3G-PG-C3B	-4.15	96.34	106.40
2	A	1995	TG1	O12-C12-C11	-3.88	124.38	128.28
2	A	1995	TG1	C7-C6-C5	3.70	124.88	115.41
3	A	1996	ACP	N3-C2-N1	-3.52	123.18	128.68
2	A	1995	TG1	C11-C7-C6	-3.32	96.63	103.03
3	A	1996	ACP	C4-C5-N7	3.19	112.73	109.40
2	A	1995	TG1	C24-C22-C21	3.19	133.41	120.78
2	A	1995	TG1	O5-C12-O12	3.16	125.81	121.62
3	A	1996	ACP	PB-O3A-PA	3.03	142.18	132.56
3	A	1996	ACP	O2A-PA-O5'	2.86	121.04	107.75
3	A	1996	ACP	O2B-PB-C3B	2.79	117.98	106.58
2	A	1995	TG1	C23-C22-C21	-2.66	109.44	116.09
3	A	1996	ACP	O1B-PB-C3B	-2.08	103.58	109.07
2	A	1995	TG1	C2-O1-C13	-2.05	114.12	117.53
3	A	1996	ACP	O2G-PG-C3B	2.02	111.31	106.40
2	A	1995	TG1	O7-C27-O8	2.02	128.59	123.70

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1996	ACP	O4'-C4'-C5'-O5'
2	A	1995	TG1	C33-C32-O9-C10
2	A	1995	TG1	O10-C32-O9-C10
2	A	1995	TG1	C13-C14-C15-C16
2	A	1995	TG1	C14-C15-C16-C17
2	A	1995	TG1	C15-C16-C17-C18
3	A	1996	ACP	C3'-C4'-C5'-O5'
2	A	1995	TG1	C16-C17-C18-C19
2	A	1995	TG1	C17-C18-C19-C20
2	A	1995	TG1	O1-C13-C14-C15

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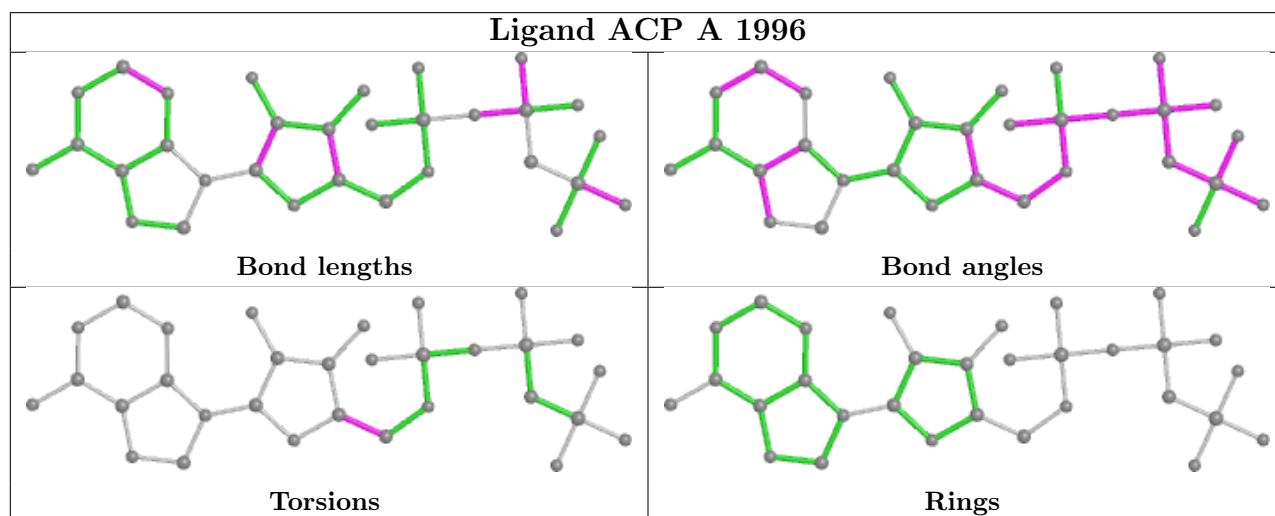
Mol	Chain	Res	Type	Atoms
2	A	1995	TG1	O3-C21-C22-C23
2	A	1995	TG1	O4-C21-C22-C23
2	A	1995	TG1	O2-C13-C14-C15
2	A	1995	TG1	O7-C27-C28-C29

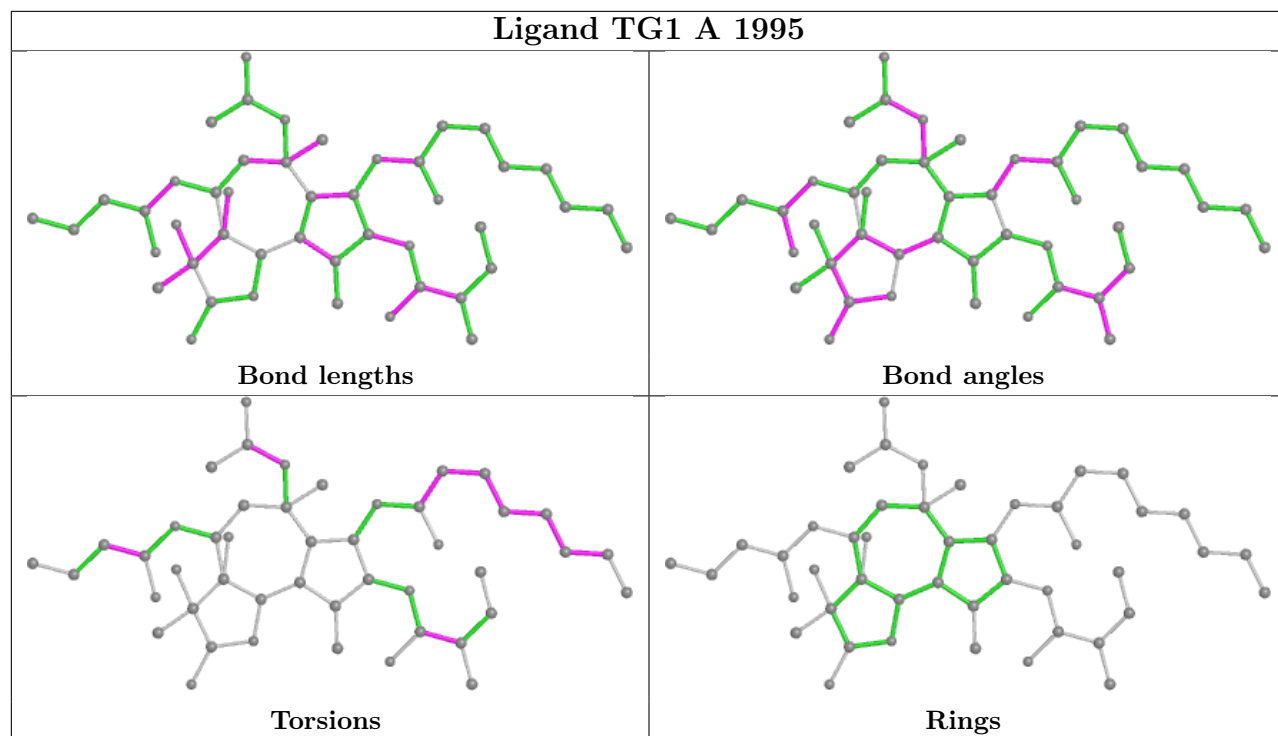
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1996	ACP	9	0
2	A	1995	TG1	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	994/994 (100%)	0.08	69 (6%) 16 10	16, 59, 133, 185	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	994	GLY	11.1
1	A	877	THR	8.6
1	A	286	GLY	8.0
1	A	881	PRO	6.9
1	A	992	LEU	6.3
1	A	878	GLU	5.6
1	A	505	ARG	5.6
1	A	281	ASP	5.4
1	A	80	GLU	5.4
1	A	507	ALA	5.0
1	A	78	PHE	4.7
1	A	964	LEU	4.6
1	A	993	GLU	4.4
1	A	184	SER	4.4
1	A	283	VAL	4.4
1	A	82	GLU	4.3
1	A	46	GLY	4.2
1	A	84	THR	4.2
1	A	1	MET	3.9
1	A	504	SER	3.9
1	A	957	PHE	3.8
1	A	81	GLY	3.8
1	A	876	CYS	3.8
1	A	47	LYS	3.8
1	A	963	ASP	3.7
1	A	284	HIS	3.7
1	A	427	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	879	ASP	3.6
1	A	951	ASP	3.6
1	A	959	LEU	3.6
1	A	503	SER	3.5
1	A	880	HIS	3.4
1	A	991	TYR	3.4
1	A	924	ARG	3.3
1	A	767	SER	3.2
1	A	888	CYS	3.2
1	A	928	TRP	3.2
1	A	109	GLU	3.2
1	A	502	LYS	3.0
1	A	960	LYS	3.0
1	A	50	TRP	3.0
1	A	433	VAL	3.0
1	A	285	GLY	3.0
1	A	287	SER	2.8
1	A	461	ASN	2.8
1	A	435	GLU	2.8
1	A	886	LEU	2.8
1	A	280	ASN	2.7
1	A	428	ASN	2.7
1	A	282	PRO	2.7
1	A	861	ASP	2.6
1	A	110	ARG	2.6
1	A	768	ASN	2.6
1	A	111	ASN	2.5
1	A	113	GLU	2.5
1	A	288	TRP	2.3
1	A	949	TYR	2.3
1	A	920	GLN	2.3
1	A	54	ILE	2.2
1	A	290	ARG	2.2
1	A	923	MET	2.2
1	A	782	GLY	2.2
1	A	77	TRP	2.2
1	A	508	VAL	2.1
1	A	106	VAL	2.1
1	A	79	GLU	2.1
1	A	305	ALA	2.1
1	A	509	GLY	2.0
1	A	430	THR	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 monosaccharides in this entry.

6.4 Ligands [i](#)

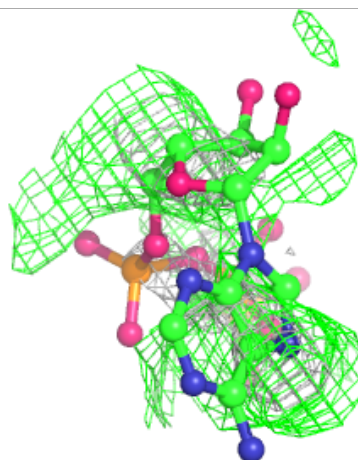
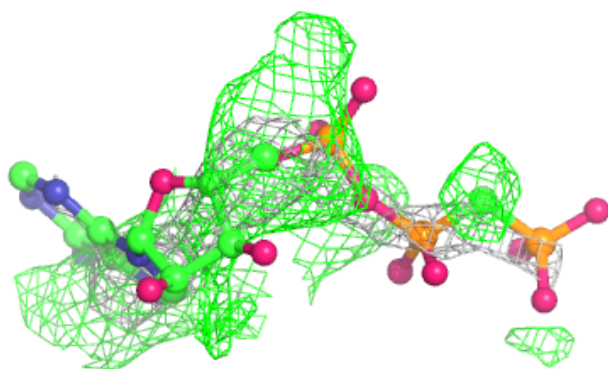
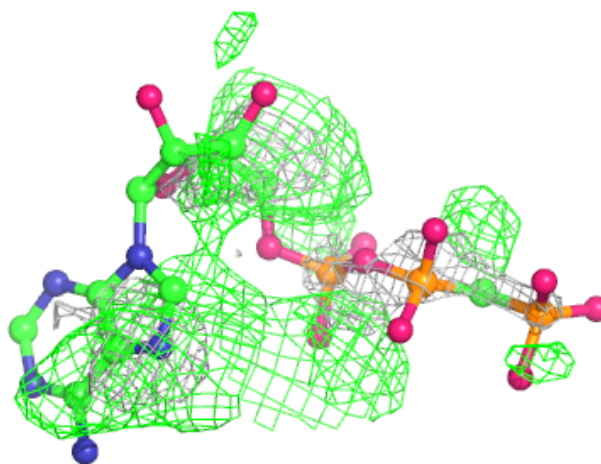
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

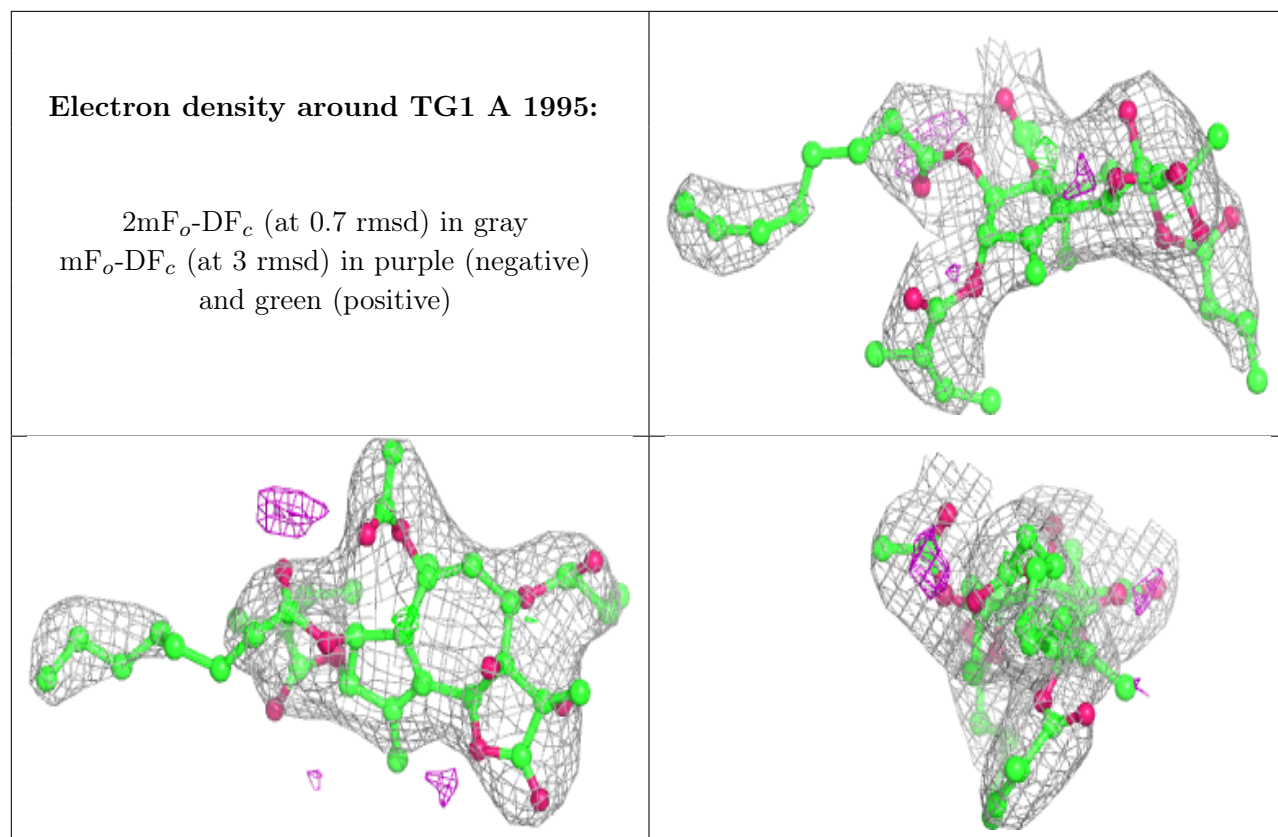
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACP	A	1996	31/31	0.63	0.54	29,33,36,36	31
4	MG	A	1997	1/1	0.84	2.02	66,66,66,66	1
2	TG1	A	1995	46/46	0.93	0.23	63,74,89,89	0
5	NA	A	1998	1/1	0.94	0.22	41,41,41,41	0

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.