



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:12 AM UTC

PDB ID : 2C8L / pdb_00002c8l
Title : Crystal Structure of (SR) Calcium-ATPase E2(Tg) form
Authors : Jensen, A.M.; Sorensen, T.L.; Olesen, C.; Moller, J.V.; Nissen, P.
Deposited on : 2005-12-06
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

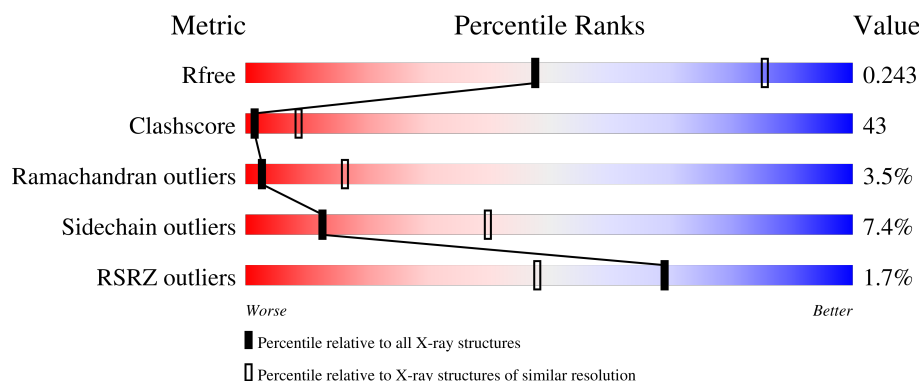
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

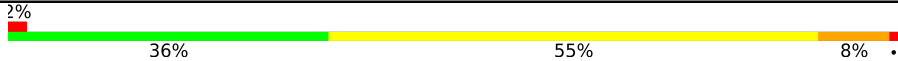
The reported resolution of this entry is 3.10 Å.

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 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	

2 Entry composition [i](#)

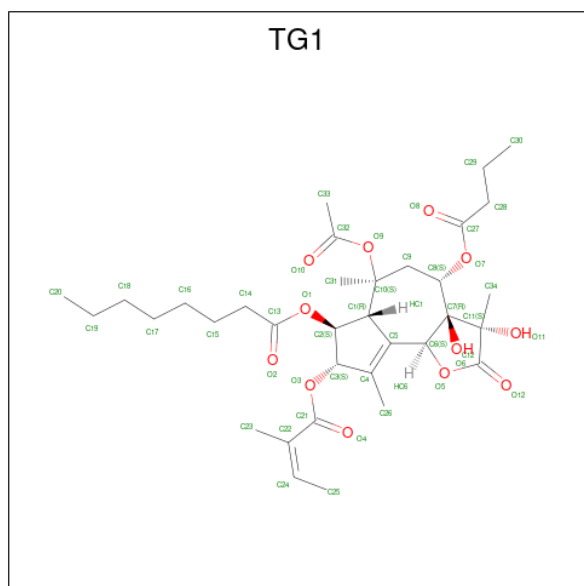
There are 3 unique types of molecules in this entry. The entry contains 7718 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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 (CCD ID: TG1) (formula: C₃₄H₅₀O₁₂).



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

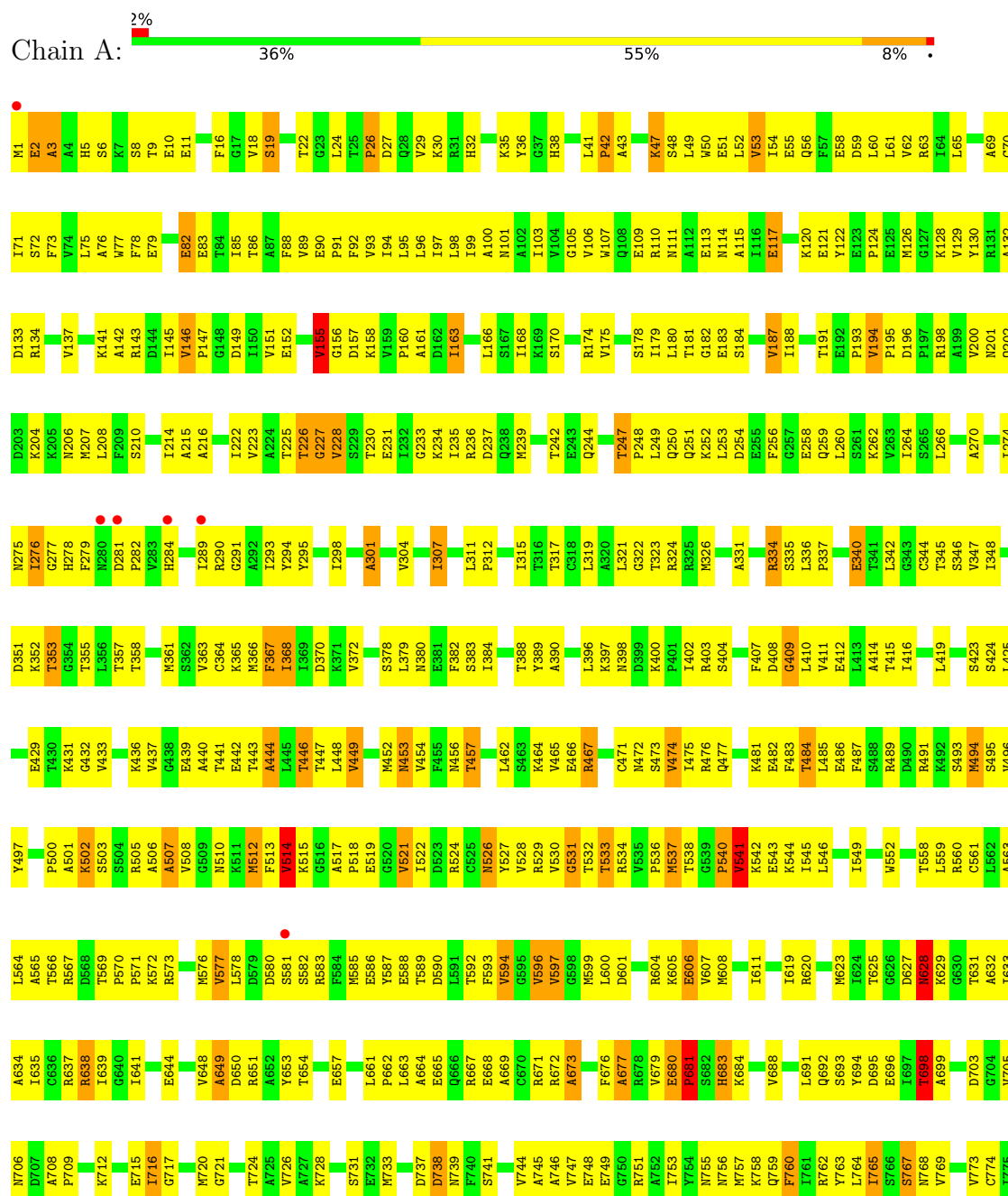
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

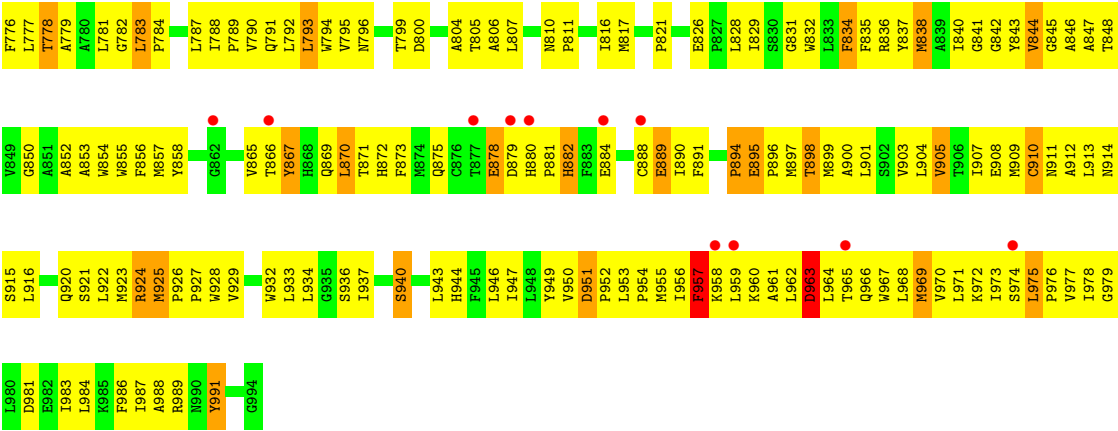
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0

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: SARCOPLASMIC/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	71.51Å 71.51Å 589.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 3.10 14.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (14.99-3.10) 98.7 (14.99-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.306 0.248 , 0.243	Depositor DCC
R_{free} test set	1496 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	76.6	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7718	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.52	0/7812	1.04	40/10592 (0.4%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ALA	N-CA-C	-9.86	98.29	110.61
1	A	157	ASP	N-CA-C	9.82	123.01	110.24
1	A	641	ILE	N-CA-C	-9.19	100.99	111.00
1	A	301	ALA	N-CA-C	-7.47	102.74	111.03
1	A	601	ASP	CA-C-N	7.31	127.91	120.38
1	A	601	ASP	C-N-CA	7.31	127.91	120.38
1	A	698	THR	N-CA-C	7.12	121.00	109.40
1	A	486	GLU	N-CA-C	7.02	119.62	110.43
1	A	838	MET	N-CA-C	-6.99	103.75	111.36
1	A	2	GLU	N-CA-C	6.96	125.62	110.80
1	A	867	TYR	N-CA-C	-6.61	104.96	113.16
1	A	121	GLU	N-CA-C	-6.54	105.21	113.72
1	A	924	ARG	N-CA-C	-6.40	105.49	113.55
1	A	721	GLY	N-CA-C	-6.38	105.11	112.50
1	A	514	VAL	N-CA-C	6.28	117.52	108.48
1	A	307	ILE	N-CA-C	6.18	115.00	108.95
1	A	163	ILE	N-CA-C	6.14	116.77	108.17
1	A	444	ALA	N-CA-C	-6.05	103.43	111.24
1	A	510	ASN	N-CA-C	6.05	119.04	109.96
1	A	852	ALA	N-CA-C	-5.80	104.38	112.45
1	A	155	VAL	N-CA-C	5.75	121.29	109.34
1	A	806	ALA	N-CA-C	-5.72	104.96	111.14
1	A	680	GLU	CA-C-N	5.70	126.97	119.84
1	A	680	GLU	C-N-CA	5.70	126.97	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	969	MET	N-CA-C	-5.63	104.83	110.97
1	A	194	VAL	CA-C-N	5.61	126.85	119.84
1	A	194	VAL	C-N-CA	5.61	126.85	119.84
1	A	632	ALA	N-CA-C	-5.58	105.10	111.07
1	A	834	PHE	N-CA-C	-5.58	105.10	111.07
1	A	467	ARG	N-CA-C	-5.39	106.54	113.01
1	A	673	ALA	N-CA-C	5.38	117.82	110.24
1	A	27	ASP	N-CA-C	-5.35	105.09	111.03
1	A	628	ASN	N-CA-C	-5.21	103.27	110.35
1	A	767	SER	N-CA-C	-5.14	105.36	110.97
1	A	251	GLN	N-CA-C	-5.09	105.64	111.14
1	A	276	ILE	N-CA-C	-5.09	106.94	112.80
1	A	334	ARG	N-CA-C	-5.09	101.41	109.96
1	A	351	ASP	N-CA-C	-5.07	103.36	110.50
1	A	890	ILE	N-CA-C	-5.04	104.80	111.09
1	A	526	ASN	N-CA-C	-5.01	107.15	114.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7671	0	7764	674	0
2	A	46	0	50	5	0
3	A	1	0	0	0	0
All	All	7718	0	7814	674	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 43.

All (674) 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:898:THR:HG22	1:A:958:LYS:HB3	1.26	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASN:HB3	1:A:471:CYS:SG	1.94	1.07
1:A:795:VAL:HA	1:A:799:THR:OG1	1.55	1.05
1:A:484:THR:HB	1:A:496:VAL:HG12	1.39	1.04
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.22	1.03
1:A:298:ILE:HD11	1:A:779:ALA:HB2	1.44	0.99
1:A:865:VAL:HG11	1:A:869:GLN:HB2	1.41	0.99
1:A:436:LYS:HG3	1:A:443:THR:HG21	1.41	0.99
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.43	0.99
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.44	0.98
1:A:388:THR:HG22	1:A:390:ALA:H	1.28	0.98
1:A:879:ASP:OD1	1:A:882:HIS:HB3	1.64	0.98
1:A:680:GLU:H	1:A:683:HIS:HD2	1.08	0.97
1:A:227:GLY:O	1:A:230:THR:HG22	1.65	0.96
1:A:361:MET:HE2	1:A:441:THR:HG22	1.47	0.96
1:A:342:LEU:O	1:A:345:THR:HG23	1.67	0.95
1:A:411:VAL:HG12	1:A:454:VAL:HB	1.47	0.94
1:A:397:LYS:O	1:A:400:LYS:HG2	1.67	0.93
1:A:301:ALA:HA	1:A:789:PRO:HG3	1.50	0.93
1:A:606:GLU:H	1:A:606:GLU:CD	1.76	0.93
1:A:527:TYR:HB2	1:A:592:THR:HG22	1.48	0.93
1:A:759:GLN:HE22	1:A:762:ARG:HH11	1.07	0.93
1:A:1:MET:HG2	1:A:225:THR:HG22	1.49	0.91
1:A:100:ALA:HA	1:A:103:ILE:HD12	1.50	0.91
1:A:654:THR:HG22	1:A:657:GLU:HG3	1.53	0.90
1:A:751:ARG:HD2	1:A:817:MET:HE1	1.53	0.89
1:A:439:GLU:O	1:A:443:THR:HG22	1.72	0.87
1:A:247:THR:HG23	1:A:340:GLU:OE1	1.72	0.87
1:A:99:ILE:HG22	1:A:103:ILE:HD11	1.56	0.86
1:A:759:GLN:HE22	1:A:762:ARG:NH1	1.73	0.86
1:A:969:MET:HG3	1:A:973:ILE:HD11	1.57	0.86
1:A:959:LEU:HG	1:A:960:LYS:HG2	1.58	0.86
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.56	0.86
1:A:278:HIS:C	1:A:282:PRO:HG3	2.02	0.85
1:A:909:MET:HE3	1:A:937:ILE:HG23	1.58	0.85
1:A:751:ARG:HD2	1:A:817:MET:CE	2.07	0.84
1:A:355:THR:HG22	1:A:738:ASP:O	1.77	0.83
1:A:733:MET:HE1	1:A:746:ALA:CB	2.08	0.83
1:A:925:MET:HE1	1:A:929:VAL:HG11	1.61	0.83
1:A:331:ALA:HB1	1:A:733:MET:HE2	1.60	0.82
1:A:161:ALA:HA	1:A:210:SER:HB2	1.61	0.82
1:A:898:THR:CG2	1:A:958:LYS:HB3	2.08	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.62	0.81
1:A:315:ILE:HG23	1:A:757:MET:HE2	1.63	0.81
1:A:26:PRO:O	1:A:30:LYS:HD3	1.81	0.81
1:A:951:ASP:O	1:A:954:PRO:HD2	1.81	0.81
1:A:563:ALA:O	1:A:564:LEU:HD23	1.81	0.81
1:A:180:LEU:HA	1:A:705:VAL:HG12	1.64	0.80
1:A:436:LYS:CG	1:A:443:THR:HG21	2.11	0.80
1:A:254:ASP:O	1:A:258:GLU:HG2	1.82	0.80
1:A:49:LEU:HA	1:A:52:LEU:HD12	1.64	0.79
1:A:89:VAL:O	1:A:93:VAL:HG23	1.82	0.79
1:A:95:LEU:O	1:A:99:ILE:HG12	1.83	0.79
1:A:414:ALA:HB2	1:A:452:MET:HE2	1.61	0.79
1:A:828:LEU:HD12	2:A:1995:TG1:H302	1.64	0.79
1:A:623:MET:HE1	1:A:635:ILE:HG22	1.63	0.78
1:A:398:ASN:HB2	1:A:400:LYS:NZ	1.99	0.78
1:A:880:HIS:HB3	1:A:881:PRO:HD3	1.65	0.78
1:A:230:THR:HG23	1:A:233:GLY:H	1.49	0.78
1:A:911:ASN:HA	1:A:914:ASN:ND2	1.97	0.77
1:A:680:GLU:H	1:A:683:HIS:CD2	1.98	0.77
1:A:352:LYS:CB	1:A:625:THR:HG22	2.15	0.77
1:A:898:THR:HG22	1:A:958:LYS:CB	2.13	0.76
1:A:933:LEU:O	1:A:937:ILE:HG13	1.85	0.76
1:A:252:LYS:HE2	1:A:826:GLU:O	1.85	0.76
1:A:200:VAL:HG21	1:A:489:ARG:HH22	1.49	0.76
1:A:398:ASN:HB2	1:A:400:LYS:HZ3	1.51	0.76
1:A:895:GLU:HA	1:A:898:THR:HG23	1.66	0.76
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.26	0.75
1:A:248:PRO:O	1:A:252:LYS:HG3	1.87	0.75
1:A:914:ASN:HB3	1:A:981:ASP:OD2	1.85	0.75
1:A:247:THR:HG22	1:A:250:GLN:HG3	1.67	0.75
1:A:352:LYS:HB2	1:A:625:THR:HG22	1.66	0.75
1:A:415:THR:HA	1:A:475:ILE:HG21	1.69	0.75
1:A:901:LEU:HD22	1:A:958:LYS:NZ	2.02	0.75
1:A:654:THR:HG22	1:A:657:GLU:CG	2.15	0.74
1:A:397:LYS:HB2	1:A:402:ILE:HD11	1.69	0.74
1:A:932:TRP:HA	1:A:932:TRP:CE3	2.22	0.74
1:A:989:ARG:C	1:A:991:TYR:H	1.94	0.73
1:A:244:GLN:CD	1:A:244:GLN:H	1.95	0.73
1:A:531:GLY:O	1:A:533:THR:HG23	1.87	0.73
1:A:950:VAL:O	1:A:954:PRO:HG2	1.88	0.73
1:A:865:VAL:HG11	1:A:869:GLN:CB	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:MET:HE1	1:A:746:ALA:HB1	1.68	0.73
1:A:334:ARG:O	1:A:335:SER:HB3	1.88	0.73
1:A:526:ASN:ND2	1:A:590:ASP:HA	2.03	0.72
1:A:352:LYS:HE2	1:A:627:ASP:OD2	1.89	0.72
1:A:529:ARG:HG3	1:A:533:THR:O	1.89	0.72
1:A:408:ASP:O	1:A:411:VAL:HG22	1.88	0.72
1:A:388:THR:HG22	1:A:390:ALA:N	2.04	0.72
1:A:880:HIS:O	1:A:884:GLU:HB2	1.89	0.71
1:A:651:ARG:HG2	1:A:651:ARG:HH11	1.53	0.71
1:A:397:LYS:CB	1:A:402:ILE:HD11	2.21	0.71
1:A:654:THR:CG2	1:A:657:GLU:HG3	2.20	0.71
1:A:974:SER:O	1:A:977:VAL:HG23	1.91	0.71
1:A:680:GLU:N	1:A:683:HIS:HD2	1.85	0.70
1:A:577:VAL:HB	1:A:580:ASP:OD1	1.90	0.70
1:A:608:MET:SD	1:A:639:ILE:HA	2.31	0.70
1:A:720:MET:HB3	1:A:738:ASP:OD1	1.92	0.70
1:A:921:SER:OG	1:A:923:MET:HG2	1.91	0.70
1:A:962:LEU:HB3	1:A:966:GLN:HG3	1.74	0.70
1:A:926:PRO:HG2	1:A:929:VAL:HG23	1.74	0.70
1:A:415:THR:HG22	1:A:475:ILE:HG23	1.74	0.69
1:A:19:SER:OG	1:A:22:THR:HB	1.92	0.69
1:A:526:ASN:HD22	1:A:590:ASP:HA	1.57	0.69
1:A:317:THR:O	1:A:321:LEU:HG	1.92	0.69
1:A:201:ASN:HA	1:A:204:LYS:HD2	1.75	0.69
1:A:680:GLU:HB3	1:A:681:PRO:CD	2.20	0.69
1:A:59:ASP:O	1:A:62:VAL:HG12	1.92	0.69
1:A:247:THR:HG22	1:A:250:GLN:H	1.58	0.69
1:A:298:ILE:CD1	1:A:779:ALA:HB2	2.21	0.69
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.21	0.69
1:A:909:MET:HE3	1:A:937:ILE:CG2	2.23	0.69
1:A:756:ASN:OD1	1:A:810:ASN:HB2	1.92	0.69
1:A:901:LEU:HD13	1:A:958:LYS:HZ1	1.58	0.68
1:A:527:TYR:O	1:A:592:THR:HA	1.94	0.68
1:A:431:LYS:O	1:A:433:VAL:HG23	1.93	0.68
1:A:77:TRP:C	1:A:79:GLU:H	2.01	0.67
1:A:82:GLU:OE2	1:A:83:GLU:HG3	1.94	0.67
1:A:512:MET:HE1	1:A:571:PRO:HD2	1.76	0.67
1:A:950:VAL:HG12	1:A:951:ASP:N	2.10	0.67
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.76	0.67
1:A:623:MET:HE1	1:A:635:ILE:CG2	2.24	0.67
1:A:115:ALA:HB3	1:A:239:MET:HE1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:GLU:CD	1:A:519:GLU:H	2.03	0.67
1:A:522:ILE:HG22	1:A:542:LYS:HE3	1.74	0.67
1:A:950:VAL:CG1	1:A:951:ASP:N	2.59	0.66
1:A:969:MET:HE3	1:A:972:LYS:HG3	1.76	0.66
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.61	0.66
1:A:166:LEU:HD11	1:A:222:ILE:HB	1.77	0.66
1:A:319:LEU:HD21	1:A:757:MET:HE1	1.76	0.66
1:A:411:VAL:HA	1:A:454:VAL:CG1	2.24	0.65
1:A:757:MET:HA	1:A:760:PHE:CE2	2.31	0.65
1:A:59:ASP:HB3	1:A:62:VAL:HG12	1.77	0.65
1:A:281:ASP:N	1:A:282:PRO:HD2	2.12	0.65
1:A:319:LEU:CD2	1:A:757:MET:HE1	2.27	0.65
1:A:69:ALA:HB2	1:A:94:ILE:HG21	1.78	0.65
1:A:471:CYS:O	1:A:474:VAL:HG22	1.97	0.65
1:A:528:VAL:HG12	1:A:593:PHE:HB3	1.77	0.65
1:A:835:PHE:O	1:A:838:MET:HB3	1.97	0.65
1:A:901:LEU:CD1	1:A:958:LYS:HZ1	2.10	0.65
1:A:855:TRP:CE3	1:A:896:PRO:HB3	2.32	0.64
1:A:781:LEU:C	1:A:783:LEU:H	2.06	0.64
1:A:512:MET:HE3	1:A:570:PRO:CB	2.27	0.64
1:A:969:MET:O	1:A:973:ILE:HG13	1.97	0.64
1:A:75:LEU:HD22	1:A:293:ILE:HG13	1.79	0.64
1:A:304:VAL:HG21	1:A:789:PRO:HA	1.79	0.64
1:A:932:TRP:HA	1:A:932:TRP:HE3	1.59	0.63
1:A:161:ALA:CA	1:A:210:SER:HB2	2.27	0.63
1:A:473:SER:O	1:A:477:GLN:HG3	1.98	0.63
1:A:900:ALA:O	1:A:903:VAL:HG12	1.98	0.63
1:A:361:MET:HE3	1:A:599:MET:HG3	1.79	0.63
1:A:24:LEU:HD13	1:A:149:ASP:HA	1.80	0.63
1:A:347:VAL:HG22	1:A:620:ARG:HB3	1.79	0.63
1:A:32:HIS:CB	1:A:146:VAL:HG11	2.28	0.63
1:A:737:ASP:OD2	1:A:739:ASN:HB2	1.99	0.62
1:A:661:LEU:HD13	1:A:665:GLU:HG3	1.81	0.62
1:A:72:SER:OG	1:A:91:PRO:HG3	1.98	0.62
1:A:100:ALA:HA	1:A:103:ILE:CD1	2.28	0.62
1:A:530:VAL:O	1:A:530:VAL:HG23	1.98	0.62
1:A:870:LEU:HD12	1:A:870:LEU:O	1.98	0.62
1:A:606:GLU:CD	1:A:606:GLU:N	2.53	0.62
1:A:436:LYS:HG3	1:A:443:THR:CG2	2.22	0.62
1:A:85:ILE:HG13	1:A:85:ILE:O	1.99	0.62
1:A:99:ILE:O	1:A:103:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ALA:O	1:A:502:LYS:HB2	1.99	0.62
1:A:795:VAL:HA	1:A:799:THR:HG1	1.60	0.62
1:A:397:LYS:HG3	1:A:398:ASN:HD22	1.65	0.61
1:A:563:ALA:C	1:A:564:LEU:HD23	2.24	0.61
1:A:397:LYS:HB2	1:A:402:ILE:CD1	2.31	0.61
1:A:527:TYR:HB2	1:A:592:THR:CG2	2.28	0.61
1:A:122:TYR:HE2	1:A:726:VAL:HG21	1.65	0.61
1:A:404:SER:OG	1:A:452:MET:HB2	2.01	0.61
1:A:909:MET:HE1	1:A:940:SER:HB2	1.83	0.61
1:A:951:ASP:HB3	1:A:952:PRO:HD3	1.83	0.61
1:A:607:VAL:O	1:A:611:ILE:HG12	2.00	0.61
1:A:370:ASP:HB2	1:A:379:LEU:O	2.00	0.60
1:A:788:ILE:HG22	1:A:790:VAL:H	1.66	0.60
1:A:679:VAL:HG13	1:A:683:HIS:CB	2.31	0.60
1:A:247:THR:CG2	1:A:250:GLN:HG3	2.30	0.60
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.83	0.60
1:A:47:LYS:HD3	1:A:51:GLU:HB3	1.84	0.60
1:A:748:GLU:HA	1:A:817:MET:HE3	1.83	0.60
1:A:402:ILE:HG22	1:A:403:ARG:N	2.17	0.60
1:A:963:ASP:O	1:A:967:TRP:HB2	2.00	0.60
1:A:99:ILE:HG22	1:A:103:ILE:CD1	2.32	0.60
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.84	0.60
1:A:903:VAL:O	1:A:907:ILE:HG13	2.02	0.60
1:A:495:SER:HB3	1:A:514:VAL:HB	1.83	0.60
1:A:628:ASN:N	1:A:628:ASN:HD22	1.99	0.60
1:A:637:ARG:HD3	1:A:644:GLU:HA	1.83	0.60
1:A:536:PRO:O	1:A:538:THR:HG23	2.02	0.59
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.37	0.59
1:A:389:TYR:CE2	1:A:436:LYS:HB2	2.37	0.59
1:A:951:ASP:C	1:A:954:PRO:HD2	2.27	0.59
1:A:47:LYS:HB3	1:A:51:GLU:HB2	1.85	0.59
1:A:505:ARG:HG3	1:A:505:ARG:O	2.03	0.59
1:A:749:GLU:O	1:A:753:ILE:HG12	2.02	0.59
1:A:518:PRO:HA	1:A:563:ALA:HB2	1.85	0.59
1:A:361:MET:HE3	1:A:599:MET:HE2	1.84	0.59
1:A:909:MET:HE3	1:A:937:ILE:HA	1.84	0.59
1:A:452:MET:O	1:A:453:ASN:C	2.46	0.59
1:A:18:VAL:CG2	1:A:24:LEU:HD12	2.33	0.59
1:A:248:PRO:HG2	1:A:340:GLU:OE2	2.04	0.58
1:A:281:ASP:N	1:A:282:PRO:CD	2.66	0.58
1:A:964:LEU:C	1:A:966:GLN:H	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:PHE:HE1	1:A:485:LEU:HD21	1.67	0.58
1:A:512:MET:CE	1:A:571:PRO:HD2	2.33	0.58
1:A:545:ILE:O	1:A:549:ILE:HG12	2.03	0.58
1:A:565:ALA:HA	1:A:594:VAL:HG13	1.84	0.58
1:A:765:ILE:O	1:A:769:VAL:HG23	2.04	0.58
1:A:946:LEU:HD12	1:A:950:VAL:HG23	1.85	0.58
1:A:974:SER:C	1:A:976:PRO:HD2	2.28	0.58
1:A:909:MET:HB3	1:A:937:ILE:CG2	2.34	0.58
1:A:126:MET:SD	1:A:141:LYS:HG2	2.43	0.58
1:A:716:ILE:HD12	1:A:716:ILE:N	2.18	0.58
1:A:909:MET:HB3	1:A:937:ILE:HG23	1.85	0.58
1:A:482:GLU:HG3	1:A:497:TYR:HD2	1.69	0.58
1:A:840:ILE:O	1:A:844:VAL:HG12	2.03	0.58
1:A:895:GLU:N	1:A:896:PRO:HD2	2.19	0.58
1:A:32:HIS:HB3	1:A:146:VAL:CG1	2.34	0.57
1:A:92:PHE:CE2	1:A:96:LEU:HD11	2.39	0.57
1:A:654:THR:HA	1:A:677:ALA:HB3	1.86	0.57
1:A:5:HIS:HE1	1:A:196:ASP:O	1.86	0.57
1:A:367:PHE:CD1	1:A:367:PHE:C	2.82	0.57
1:A:788:ILE:HB	1:A:791:GLN:HG3	1.86	0.57
1:A:836:ARG:O	1:A:840:ILE:HG12	2.04	0.57
1:A:955:MET:C	1:A:957:PHE:H	2.12	0.57
1:A:278:HIS:O	1:A:282:PRO:HG3	2.04	0.57
1:A:748:GLU:HA	1:A:817:MET:CE	2.35	0.57
1:A:133:ASP:O	1:A:134:ARG:HG3	2.05	0.57
1:A:530:VAL:O	1:A:531:GLY:O	2.22	0.57
1:A:326:MET:HE1	1:A:342:LEU:HD23	1.87	0.57
1:A:368:ILE:HD13	1:A:410:LEU:HD21	1.84	0.57
1:A:580:ASP:OD1	1:A:580:ASP:N	2.38	0.57
1:A:244:GLN:CD	1:A:244:GLN:N	2.63	0.57
1:A:423:SER:OG	1:A:442:GLU:HB2	2.05	0.57
1:A:47:LYS:HB3	1:A:51:GLU:CB	2.35	0.56
1:A:76:ALA:HB1	1:A:88:PHE:HD1	1.70	0.56
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.86	0.56
1:A:628:ASN:HD21	1:A:631:THR:HB	1.70	0.56
1:A:760:PHE:CD1	1:A:760:PHE:C	2.83	0.56
1:A:163:ILE:C	1:A:207:MET:HE3	2.30	0.56
1:A:957:PHE:HD1	1:A:957:PHE:O	1.88	0.56
1:A:366:MET:HG3	1:A:384:ILE:HD11	1.87	0.56
1:A:512:MET:HE3	1:A:570:PRO:HB2	1.87	0.56
1:A:436:LYS:CD	1:A:443:THR:HG21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LEU:HD22	1:A:466:GLU:OE1	2.06	0.56
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.71	0.56
1:A:2:GLU:OE1	1:A:16:PHE:HE2	1.89	0.56
1:A:793:LEU:O	1:A:794:TRP:C	2.49	0.56
1:A:943:LEU:O	1:A:946:LEU:HB3	2.06	0.56
1:A:944:HIS:C	1:A:946:LEU:H	2.12	0.56
1:A:628:ASN:HD21	1:A:631:THR:CB	2.18	0.56
1:A:18:VAL:HG22	1:A:19:SER:N	2.21	0.55
1:A:65:LEU:CD2	1:A:94:ILE:HG23	2.36	0.55
1:A:648:VAL:O	1:A:649:ALA:C	2.49	0.55
1:A:841:GLY:O	1:A:844:VAL:HG13	2.05	0.55
1:A:907:ILE:HG23	1:A:977:VAL:HG21	1.87	0.55
1:A:688:VAL:O	1:A:692:GLN:HG3	2.05	0.55
1:A:319:LEU:CG	1:A:757:MET:HE1	2.37	0.55
1:A:848:THR:HG22	1:A:903:VAL:HG13	1.89	0.55
1:A:6:SER:HA	1:A:194:VAL:O	2.07	0.55
1:A:38:HIS:CE1	1:A:143:ARG:HH12	2.25	0.55
1:A:950:VAL:CG1	1:A:951:ASP:H	2.20	0.55
1:A:122:TYR:O	1:A:158:LYS:HD3	2.06	0.55
1:A:751:ARG:HD2	1:A:817:MET:HE2	1.89	0.54
1:A:235:ILE:HG23	1:A:709:PRO:HD3	1.89	0.54
1:A:322:GLY:O	1:A:326:MET:HG3	2.06	0.54
1:A:777:LEU:O	1:A:778:THR:C	2.50	0.54
1:A:319:LEU:HG	1:A:757:MET:HE1	1.90	0.54
1:A:508:VAL:HG12	1:A:508:VAL:O	2.07	0.54
1:A:843:TYR:CE2	1:A:977:VAL:HG22	2.43	0.54
1:A:901:LEU:HD22	1:A:958:LYS:HZ3	1.72	0.54
1:A:559:LEU:HD23	1:A:600:LEU:HB2	1.88	0.54
1:A:628:ASN:ND2	1:A:631:THR:H	2.06	0.54
1:A:783:LEU:HD21	1:A:853:ALA:HB2	1.90	0.54
1:A:901:LEU:CD2	1:A:958:LYS:HZ1	2.21	0.54
1:A:32:HIS:HB2	1:A:146:VAL:HG11	1.90	0.53
1:A:98:LEU:O	1:A:101:ASN:HB2	2.08	0.53
1:A:181:THR:OG1	1:A:183:GLU:HG2	2.07	0.53
1:A:383:SER:C	1:A:384:ILE:HD12	2.33	0.53
1:A:408:ASP:O	1:A:409:GLY:C	2.51	0.53
1:A:19:SER:HG	1:A:22:THR:HB	1.73	0.53
1:A:151:VAL:HG12	1:A:152:GLU:N	2.24	0.53
1:A:278:HIS:HA	1:A:282:PRO:HD3	1.89	0.53
1:A:605:LYS:HB2	1:A:606:GLU:OE2	2.08	0.53
1:A:50:TRP:CE2	1:A:54:ILE:HD11	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD2	1:A:61:LEU:HB2	2.09	0.53
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.91	0.53
1:A:397:LYS:HG3	1:A:398:ASN:ND2	2.23	0.53
1:A:114:ASN:OD1	1:A:117:GLU:HB3	2.08	0.53
1:A:901:LEU:HD22	1:A:958:LYS:HZ1	1.74	0.53
1:A:989:ARG:C	1:A:991:TYR:N	2.65	0.53
1:A:363:VAL:HG13	1:A:597:VAL:HG13	1.90	0.53
1:A:840:ILE:O	1:A:843:TYR:HB3	2.08	0.53
1:A:954:PRO:O	1:A:957:PHE:O	2.27	0.53
1:A:442:GLU:O	1:A:446:THR:HG23	2.08	0.53
1:A:534:ARG:HD2	1:A:592:THR:HG21	1.89	0.53
1:A:242:THR:CG2	1:A:712:LYS:HZ2	2.22	0.53
1:A:979:GLY:O	1:A:983:ILE:HG13	2.09	0.53
1:A:962:LEU:HB3	1:A:966:GLN:CG	2.40	0.52
1:A:196:ASP:OD1	1:A:198:ARG:N	2.41	0.52
1:A:352:LYS:HB3	1:A:625:THR:HG22	1.90	0.52
1:A:389:TYR:HB3	1:A:425:LEU:HD21	1.91	0.52
1:A:965:THR:H	1:A:968:LEU:HD12	1.74	0.52
1:A:8:SER:OG	1:A:11:GLU:HG3	2.09	0.52
1:A:128:LYS:HB3	1:A:137:VAL:HG21	1.90	0.52
1:A:239:MET:O	1:A:242:THR:HG22	2.09	0.52
1:A:633:ILE:HG22	1:A:637:ARG:NH1	2.23	0.52
1:A:77:TRP:C	1:A:79:GLU:N	2.67	0.52
1:A:546:LEU:O	1:A:549:ILE:HB	2.10	0.52
1:A:558:THR:HG22	1:A:634:ALA:HB1	1.90	0.52
1:A:146:VAL:HG13	1:A:147:PRO:HD2	1.92	0.52
1:A:183:GLU:O	1:A:183:GLU:HG3	2.07	0.52
1:A:848:THR:HA	1:A:903:VAL:HG11	1.91	0.52
1:A:415:THR:HG22	1:A:475:ILE:CG2	2.39	0.52
1:A:441:THR:HG21	1:A:560:ARG:NH1	2.25	0.52
1:A:878:GLU:C	1:A:880:HIS:H	2.18	0.52
1:A:388:THR:HG22	1:A:389:TYR:N	2.23	0.52
1:A:256:PHE:HB2	2:A:1995:TG1:H291	1.91	0.51
1:A:831:GLY:O	1:A:834:PHE:HB3	2.09	0.51
1:A:29:VAL:HG12	1:A:30:LYS:HD2	1.91	0.51
1:A:70:CYS:O	1:A:73:PHE:N	2.43	0.51
1:A:141:LYS:O	1:A:142:ALA:C	2.53	0.51
1:A:353:THR:HA	1:A:357:THR:OG1	2.10	0.51
1:A:532:THR:O	1:A:533:THR:HG22	2.11	0.51
1:A:964:LEU:O	1:A:966:GLN:N	2.38	0.51
1:A:41:LEU:O	1:A:42:PRO:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:GLU:HB2	1:A:741:SER:OG	2.11	0.51
1:A:961:ALA:HB3	1:A:967:TRP:NE1	2.25	0.51
1:A:361:MET:HB3	1:A:599:MET:HE2	1.91	0.51
1:A:628:ASN:ND2	1:A:628:ASN:O	2.44	0.51
1:A:654:THR:CG2	1:A:657:GLU:H	2.24	0.51
1:A:291:GLY:O	1:A:294:TYR:HB3	2.11	0.51
1:A:604:ARG:O	1:A:607:VAL:HB	2.10	0.51
1:A:487:PHE:HA	1:A:493:SER:O	2.11	0.51
1:A:755:ASN:O	1:A:758:LYS:HB3	2.11	0.51
1:A:781:LEU:O	1:A:871:THR:HG23	2.11	0.51
1:A:370:ASP:HB3	1:A:378:SER:OG	2.11	0.50
1:A:412:GLU:CD	1:A:529:ARG:HE	2.20	0.50
1:A:2:GLU:OE1	1:A:16:PHE:CE2	2.64	0.50
1:A:77:TRP:O	1:A:79:GLU:N	2.37	0.50
1:A:130:TYR:CE2	1:A:137:VAL:HB	2.47	0.50
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.92	0.50
1:A:202:GLN:HB3	1:A:489:ARG:NH2	2.27	0.50
1:A:580:ASP:O	1:A:582:SER:N	2.44	0.50
1:A:724:THR:O	1:A:728:LYS:HG3	2.11	0.50
1:A:913:LEU:C	1:A:915:SER:H	2.18	0.50
1:A:174:ARG:NE	1:A:188:ILE:HG12	2.27	0.50
1:A:397:LYS:HB3	1:A:402:ILE:HD11	1.93	0.50
1:A:855:TRP:CE2	1:A:895:GLU:HG3	2.46	0.50
1:A:857:MET:O	1:A:858:TYR:HB2	2.12	0.50
1:A:467:ARG:O	1:A:467:ARG:NH1	2.44	0.50
1:A:284:HIS:O	1:A:284:HIS:ND1	2.45	0.50
1:A:367:PHE:CD1	1:A:367:PHE:O	2.64	0.50
1:A:384:ILE:HD12	1:A:384:ILE:N	2.27	0.50
1:A:412:GLU:OE1	1:A:529:ARG:NE	2.45	0.50
1:A:696:GLU:O	1:A:698:THR:HG22	2.12	0.50
1:A:913:LEU:HD21	1:A:937:ILE:CD1	2.42	0.50
1:A:259:GLN:O	1:A:260:LEU:C	2.54	0.49
1:A:482:GLU:HG3	1:A:497:TYR:CD2	2.47	0.49
1:A:577:VAL:HB	1:A:580:ASP:CG	2.37	0.49
1:A:628:ASN:ND2	1:A:631:THR:HB	2.26	0.49
1:A:253:LEU:HD23	2:A:1995:TG1:H301	1.94	0.49
1:A:336:LEU:N	1:A:337:PRO:HD2	2.27	0.49
1:A:909:MET:CE	1:A:937:ILE:HA	2.42	0.49
1:A:179:ILE:C	1:A:179:ILE:HD12	2.38	0.49
1:A:901:LEU:CD2	1:A:958:LYS:NZ	2.75	0.49
1:A:909:MET:HE1	1:A:940:SER:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:CYS:SG	1:A:978:ILE:HD11	2.52	0.49
1:A:577:VAL:O	1:A:580:ASP:OD1	2.30	0.49
1:A:795:VAL:O	1:A:800:ASP:HB2	2.13	0.49
1:A:873:PHE:HB2	1:A:891:PHE:CD2	2.48	0.49
1:A:142:ALA:HA	1:A:145:ILE:CD1	2.42	0.49
1:A:522:ILE:CG2	1:A:542:LYS:HE3	2.41	0.49
1:A:748:GLU:HG3	1:A:817:MET:HE3	1.93	0.49
1:A:984:LEU:HA	1:A:987:ILE:HG12	1.94	0.49
1:A:228:VAL:HG13	1:A:237:ASP:OD2	2.13	0.49
1:A:76:ALA:HB1	1:A:88:PHE:CD1	2.47	0.49
1:A:113:GLU:HB2	1:A:117:GLU:OE1	2.13	0.49
1:A:155:VAL:O	1:A:214:ILE:O	2.31	0.49
1:A:231:GLU:OE2	1:A:234:LYS:NZ	2.46	0.49
1:A:901:LEU:HD13	1:A:958:LYS:NZ	2.28	0.49
1:A:465:VAL:O	1:A:465:VAL:HG12	2.12	0.49
1:A:904:LEU:O	1:A:905:VAL:C	2.56	0.49
1:A:346:SER:OG	1:A:696:GLU:HG2	2.13	0.48
1:A:894:PRO:O	1:A:898:THR:HG23	2.12	0.48
1:A:854:TRP:CZ3	1:A:899:MET:HE2	2.47	0.48
1:A:900:ALA:O	1:A:903:VAL:CG1	2.60	0.48
1:A:180:LEU:HD23	1:A:705:VAL:CG1	2.42	0.48
1:A:411:VAL:HG12	1:A:454:VAL:CB	2.33	0.48
1:A:483:PHE:CE1	1:A:485:LEU:HD21	2.48	0.48
1:A:788:ILE:H	1:A:791:GLN:CD	2.20	0.48
1:A:32:HIS:HB3	1:A:146:VAL:HG13	1.96	0.48
1:A:59:ASP:HB3	1:A:62:VAL:CG1	2.43	0.48
1:A:491:ARG:HE	1:A:588:GLU:CD	2.22	0.48
1:A:894:PRO:C	1:A:896:PRO:HD2	2.39	0.48
1:A:49:LEU:O	1:A:53:VAL:HG23	2.13	0.48
1:A:793:LEU:O	1:A:796:ASN:N	2.47	0.48
1:A:151:VAL:CG1	1:A:152:GLU:N	2.77	0.48
1:A:202:GLN:HB3	1:A:489:ARG:HH21	1.79	0.48
1:A:668:GLU:O	1:A:671:ARG:HG2	2.13	0.48
1:A:751:ARG:NH2	1:A:821:PRO:HA	2.29	0.48
1:A:955:MET:C	1:A:957:PHE:N	2.69	0.48
1:A:737:ASP:O	1:A:739:ASN:N	2.47	0.48
1:A:897:MET:C	1:A:899:MET:N	2.70	0.48
1:A:124:PRO:HB3	1:A:158:LYS:HB3	1.95	0.47
1:A:222:ILE:HG23	1:A:222:ILE:O	2.14	0.47
1:A:276:ILE:HG13	1:A:276:ILE:O	2.14	0.47
1:A:506:ALA:O	1:A:507:ALA:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:LEU:CD1	1:A:927:PRO:HA	2.44	0.47
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.96	0.47
1:A:82:GLU:H	1:A:82:GLU:CD	2.22	0.47
1:A:452:MET:O	1:A:454:VAL:N	2.48	0.47
1:A:596:VAL:CG2	1:A:597:VAL:N	2.78	0.47
1:A:909:MET:CE	1:A:940:SER:HB2	2.44	0.47
1:A:464:LYS:C	1:A:466:GLU:H	2.22	0.47
1:A:472:ASN:O	1:A:476:ARG:HG3	2.13	0.47
1:A:93:VAL:O	1:A:96:LEU:HB2	2.15	0.47
1:A:326:MET:HE1	1:A:342:LEU:CD2	2.44	0.47
1:A:379:LEU:HD11	1:A:544:LYS:HG3	1.96	0.47
1:A:541:VAL:O	1:A:545:ILE:HG13	2.15	0.47
1:A:653:TYR:CE2	1:A:669:ALA:HB1	2.50	0.47
1:A:662:PRO:O	1:A:664:ALA:N	2.47	0.47
1:A:680:GLU:CB	1:A:681:PRO:CD	2.88	0.47
1:A:837:TYR:HB2	2:A:1995:TG1:C33	2.45	0.47
1:A:872:HIS:HB3	1:A:875:GLN:NE2	2.30	0.47
1:A:946:LEU:CD1	1:A:950:VAL:HG23	2.45	0.47
1:A:758:LYS:O	1:A:762:ARG:HG3	2.14	0.47
1:A:69:ALA:HB2	1:A:94:ILE:CG2	2.43	0.47
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.28	0.47
1:A:388:THR:CG2	1:A:389:TYR:N	2.77	0.47
1:A:500:PRO:HG3	1:A:506:ALA:HA	1.96	0.47
1:A:352:LYS:HD3	1:A:625:THR:HG21	1.96	0.47
1:A:397:LYS:O	1:A:398:ASN:C	2.55	0.47
1:A:986:PHE:C	1:A:988:ALA:H	2.22	0.47
1:A:537:MET:HE3	1:A:542:LYS:HD2	1.96	0.46
1:A:879:ASP:OD1	1:A:882:HIS:CB	2.52	0.46
1:A:832:TRP:HZ2	1:A:987:ILE:HG13	1.80	0.46
1:A:236:ARG:O	1:A:236:ARG:HG2	2.14	0.46
1:A:402:ILE:CG2	1:A:403:ARG:N	2.78	0.46
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.46	0.46
1:A:323:THR:HG22	1:A:324:ARG:N	2.31	0.46
1:A:474:VAL:CG2	1:A:475:ILE:N	2.79	0.46
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.50	0.46
1:A:950:VAL:O	1:A:954:PRO:CG	2.60	0.46
1:A:174:ARG:CB	1:A:215:ALA:HB3	2.46	0.46
1:A:512:MET:HE3	1:A:570:PRO:HB3	1.97	0.46
1:A:363:VAL:O	1:A:384:ILE:HB	2.16	0.46
1:A:505:ARG:NH1	1:A:507:ALA:HB3	2.30	0.46
1:A:589:THR:O	1:A:590:ASP:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:TYR:C	1:A:950:VAL:O	2.55	0.46
1:A:586:GLU:O	1:A:589:THR:HG23	2.15	0.46
1:A:927:PRO:HB2	1:A:934:LEU:HD21	1.97	0.46
1:A:971:LEU:C	1:A:973:ILE:H	2.23	0.46
1:A:50:TRP:O	1:A:54:ILE:HG13	2.16	0.46
1:A:363:VAL:CG1	1:A:597:VAL:HG13	2.46	0.46
1:A:436:LYS:HD2	1:A:440:ALA:HA	1.96	0.46
1:A:567:ARG:CD	1:A:570:PRO:HA	2.46	0.46
1:A:577:VAL:HG23	1:A:583:ARG:NH1	2.31	0.46
1:A:737:ASP:C	1:A:739:ASN:N	2.74	0.46
1:A:52:LEU:O	1:A:53:VAL:C	2.58	0.46
1:A:361:MET:CE	1:A:599:MET:HG3	2.43	0.46
1:A:676:PHE:HB3	1:A:679:VAL:CG2	2.46	0.46
1:A:174:ARG:CG	1:A:216:ALA:HB3	2.46	0.45
1:A:364:CYS:O	1:A:383:SER:HA	2.15	0.45
1:A:174:ARG:HG2	1:A:216:ALA:HB3	1.97	0.45
1:A:193:PRO:HA	1:A:206:ASN:ND2	2.32	0.45
1:A:448:LEU:HD12	1:A:448:LEU:O	2.16	0.45
1:A:854:TRP:CE3	1:A:899:MET:HE2	2.52	0.45
1:A:909:MET:O	1:A:913:LEU:HG	2.16	0.45
1:A:52:LEU:HD13	1:A:106:VAL:HG13	1.98	0.45
1:A:505:ARG:C	1:A:507:ALA:H	2.24	0.45
1:A:540:PRO:HG2	1:A:541:VAL:H	1.82	0.45
1:A:411:VAL:O	1:A:415:THR:HG23	2.16	0.45
1:A:776:PHE:O	1:A:777:LEU:C	2.60	0.45
1:A:850:GLY:O	1:A:854:TRP:N	2.49	0.45
1:A:857:MET:HG2	1:A:866:THR:HA	1.98	0.45
1:A:922:LEU:HD23	1:A:925:MET:O	2.16	0.45
1:A:56:GLN:OE1	1:A:105:GLY:HA3	2.17	0.45
1:A:174:ARG:HA	1:A:187:VAL:O	2.16	0.45
1:A:964:LEU:C	1:A:966:GLN:N	2.72	0.45
1:A:86:THR:HG21	1:A:955:MET:HE3	1.98	0.45
1:A:352:LYS:HD2	1:A:635:ILE:HG21	1.98	0.45
1:A:532:THR:C	1:A:533:THR:CG2	2.90	0.45
1:A:174:ARG:HB2	1:A:216:ALA:H	1.82	0.45
1:A:567:ARG:HE	1:A:570:PRO:HA	1.82	0.45
1:A:737:ASP:C	1:A:739:ASN:H	2.24	0.45
1:A:788:ILE:HG23	1:A:789:PRO:HD2	1.98	0.45
1:A:959:LEU:HD21	1:A:960:LYS:HZ3	1.82	0.45
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.52	0.45
1:A:227:GLY:O	1:A:230:THR:CG2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLN:NE2	1:A:262:LYS:HD2	2.32	0.45
1:A:372:VAL:HG13	1:A:541:VAL:HG22	1.98	0.45
1:A:442:GLU:HG2	1:A:515:LYS:NZ	2.31	0.45
1:A:442:GLU:C	1:A:444:ALA:N	2.71	0.45
1:A:846:ALA:O	1:A:847:ALA:C	2.60	0.45
1:A:950:VAL:HB	1:A:953:LEU:HD12	1.99	0.45
1:A:230:THR:O	1:A:233:GLY:N	2.50	0.44
1:A:388:THR:C	1:A:390:ALA:H	2.24	0.44
1:A:109:GLU:O	1:A:111:ASN:N	2.50	0.44
1:A:348:ILE:HA	1:A:699:ALA:HB3	1.98	0.44
1:A:518:PRO:HD3	1:A:561:CYS:O	2.18	0.44
1:A:638:ARG:HG3	1:A:638:ARG:HH11	1.82	0.44
1:A:760:PHE:C	1:A:760:PHE:HD1	2.26	0.44
1:A:178:SER:O	1:A:182:GLY:N	2.50	0.44
1:A:828:LEU:C	1:A:829:ILE:HG13	2.43	0.44
1:A:855:TRP:CZ2	1:A:895:GLU:HG3	2.52	0.44
1:A:888:CYS:O	1:A:889:GLU:HB2	2.17	0.44
1:A:947:ILE:HB	1:A:957:PHE:CE1	2.52	0.44
1:A:59:ASP:O	1:A:60:LEU:C	2.60	0.44
1:A:174:ARG:HB2	1:A:216:ALA:N	2.32	0.44
1:A:619:ILE:CD1	1:A:747:VAL:HG11	2.47	0.44
1:A:717:GLY:O	1:A:731:SER:HB2	2.17	0.44
1:A:65:LEU:HB3	1:A:98:LEU:HD21	2.00	0.44
1:A:648:VAL:O	1:A:648:VAL:HG12	2.17	0.44
1:A:651:ARG:HH11	1:A:651:ARG:CG	2.24	0.44
1:A:783:LEU:HG	1:A:784:PRO:HD2	1.98	0.44
1:A:449:VAL:HG21	1:A:472:ASN:CG	2.43	0.44
1:A:841:GLY:O	1:A:842:GLY:C	2.60	0.44
1:A:895:GLU:HA	1:A:898:THR:CG2	2.41	0.44
1:A:909:MET:HE3	1:A:937:ILE:CA	2.47	0.44
1:A:295:TYR:C	1:A:298:ILE:HG22	2.42	0.44
1:A:448:LEU:O	1:A:452:MET:HG2	2.18	0.44
1:A:967:TRP:O	1:A:970:VAL:HB	2.18	0.44
1:A:262:LYS:O	1:A:266:LEU:HG	2.18	0.43
1:A:30:LYS:N	1:A:30:LYS:CD	2.80	0.43
1:A:524:ARG:HD2	1:A:588:GLU:O	2.18	0.43
1:A:619:ILE:HD11	1:A:747:VAL:HG11	1.99	0.43
1:A:517:ALA:O	1:A:521:VAL:HG13	2.18	0.43
1:A:633:ILE:CG2	1:A:637:ARG:NH1	2.81	0.43
1:A:955:MET:O	1:A:957:PHE:N	2.51	0.43
1:A:22:THR:HG22	1:A:132:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ALA:O	1:A:447:THR:N	2.51	0.43
1:A:474:VAL:HG23	1:A:475:ILE:N	2.33	0.43
1:A:693:SER:C	1:A:695:ASP:H	2.25	0.43
1:A:307:ILE:O	1:A:768:ASN:ND2	2.51	0.43
1:A:368:ILE:HG21	1:A:410:LEU:HD23	2.00	0.43
1:A:505:ARG:O	1:A:505:ARG:CG	2.67	0.43
1:A:178:SER:HB3	1:A:184:SER:HA	2.01	0.43
1:A:226:THR:HG23	1:A:227:GLY:N	2.31	0.43
1:A:260:LEU:O	1:A:264:ILE:HG13	2.19	0.43
1:A:456:ASN:O	1:A:457:THR:C	2.62	0.43
1:A:462:LEU:HD13	1:A:466:GLU:HG2	2.01	0.43
1:A:759:GLN:NE2	1:A:762:ARG:HH11	1.91	0.43
1:A:936:SER:O	1:A:937:ILE:C	2.59	0.43
1:A:147:PRO:HG3	1:A:226:THR:HB	2.00	0.43
1:A:446:THR:O	1:A:449:VAL:HG22	2.18	0.43
1:A:540:PRO:O	1:A:543:GLU:N	2.52	0.43
1:A:792:LEU:O	1:A:795:VAL:HB	2.18	0.43
1:A:926:PRO:HB2	1:A:928:TRP:CE2	2.54	0.43
1:A:43:ALA:HA	1:A:120:LYS:NZ	2.34	0.43
1:A:99:ILE:O	1:A:100:ALA:C	2.60	0.43
1:A:540:PRO:O	1:A:541:VAL:C	2.62	0.43
1:A:142:ALA:O	1:A:143:ARG:C	2.62	0.43
1:A:388:THR:C	1:A:390:ALA:N	2.77	0.43
1:A:424:SER:O	1:A:437:VAL:HB	2.19	0.43
1:A:502:LYS:HB3	1:A:503:SER:H	1.60	0.43
1:A:788:ILE:HG22	1:A:790:VAL:N	2.32	0.43
1:A:804:ALA:O	1:A:807:LEU:HB2	2.19	0.43
1:A:905:VAL:O	1:A:908:GLU:N	2.52	0.43
1:A:178:SER:HB3	1:A:183:GLU:O	2.19	0.42
1:A:230:THR:HG23	1:A:233:GLY:N	2.26	0.42
1:A:275:ASN:HB3	1:A:278:HIS:HD2	1.84	0.42
1:A:380:ASN:O	1:A:382:PHE:CD2	2.72	0.42
1:A:913:LEU:C	1:A:915:SER:N	2.77	0.42
1:A:18:VAL:HG21	1:A:24:LEU:CD1	2.49	0.42
1:A:18:VAL:HG21	1:A:24:LEU:HD12	2.01	0.42
1:A:146:VAL:HG13	1:A:147:PRO:CD	2.49	0.42
1:A:234:LYS:O	1:A:237:ASP:HB2	2.19	0.42
1:A:429:GLU:N	1:A:429:GLU:CD	2.77	0.42
1:A:773:VAL:HB	1:A:845:GLY:HA3	2.01	0.42
1:A:895:GLU:N	1:A:896:PRO:CD	2.82	0.42
1:A:30:LYS:HD2	1:A:30:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HG11	1:A:541:VAL:HG21	2.01	0.42
1:A:567:ARG:NE	1:A:570:PRO:HA	2.33	0.42
1:A:651:ARG:HG2	1:A:651:ARG:NH1	2.27	0.42
1:A:698:THR:HG23	1:A:715:GLU:OE1	2.20	0.42
1:A:746:ALA:O	1:A:747:VAL:C	2.61	0.42
1:A:878:GLU:C	1:A:880:HIS:N	2.77	0.42
1:A:969:MET:O	1:A:970:VAL:C	2.62	0.42
1:A:680:GLU:CB	1:A:681:PRO:HD2	2.30	0.42
1:A:757:MET:HA	1:A:760:PHE:CD2	2.54	0.42
1:A:782:GLY:O	1:A:873:PHE:HE2	2.03	0.42
1:A:950:VAL:HG13	1:A:951:ASP:H	1.83	0.42
1:A:168:ILE:HG22	1:A:170:SER:O	2.19	0.42
1:A:239:MET:HE2	1:A:239:MET:HB3	1.93	0.42
1:A:365:LYS:CB	1:A:552:TRP:CH2	3.02	0.42
1:A:367:PHE:CE2	1:A:596:VAL:CG1	3.03	0.42
1:A:370:ASP:HB3	1:A:378:SER:O	2.19	0.42
1:A:751:ARG:HH21	1:A:821:PRO:HA	1.85	0.42
1:A:691:LEU:O	1:A:696:GLU:HB2	2.20	0.42
1:A:97:ILE:O	1:A:98:LEU:C	2.61	0.42
1:A:352:LYS:HD3	1:A:625:THR:CG2	2.48	0.42
1:A:708:ALA:N	1:A:709:PRO:HD2	2.35	0.42
1:A:155:VAL:HG12	1:A:156:GLY:N	2.31	0.42
1:A:270:ALA:O	1:A:274:ILE:HG12	2.20	0.42
1:A:534:ARG:HD2	1:A:592:THR:CG2	2.50	0.42
1:A:763:TYR:CZ	1:A:912:ALA:HB2	2.55	0.42
1:A:70:CYS:O	1:A:71:ILE:C	2.60	0.42
1:A:277:GLY:O	1:A:282:PRO:HD3	2.20	0.42
1:A:781:LEU:O	1:A:783:LEU:N	2.53	0.42
1:A:829:ILE:HG21	2:A:1995:TG1:H333	2.00	0.42
1:A:35:LYS:HD3	1:A:36:TYR:CZ	2.55	0.41
1:A:276:ILE:HD12	1:A:279:PHE:HD2	1.85	0.41
1:A:491:ARG:HD2	1:A:585:MET:HA	2.01	0.41
1:A:932:TRP:O	1:A:933:LEU:C	2.63	0.41
1:A:975:LEU:HB2	1:A:976:PRO:HD3	2.02	0.41
1:A:355:THR:CG2	1:A:720:MET:SD	3.08	0.41
1:A:53:VAL:O	1:A:56:GLN:HB2	2.20	0.41
1:A:115:ALA:CB	1:A:239:MET:HE1	2.48	0.41
1:A:242:THR:HG23	1:A:712:LYS:NZ	2.35	0.41
1:A:494:MET:O	1:A:514:VAL:HG23	2.20	0.41
1:A:544:LYS:HA	1:A:544:LYS:HD2	1.82	0.41
1:A:573:ARG:HH21	1:A:578:LEU:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:PRO:HG3	1:A:873:PHE:CD2	2.55	0.41
1:A:107:TRP:O	1:A:111:ASN:ND2	2.52	0.41
1:A:900:ALA:C	1:A:903:VAL:HG12	2.44	0.41
1:A:2:GLU:HB3	1:A:3:ALA:H	1.52	0.41
1:A:402:ILE:HG21	1:A:407:PHE:HE2	1.86	0.41
1:A:628:ASN:ND2	1:A:628:ASN:C	2.78	0.41
1:A:178:SER:C	1:A:180:LEU:N	2.78	0.41
1:A:247:THR:HG23	1:A:249:LEU:H	1.85	0.41
1:A:419:LEU:O	1:A:481:LYS:HE3	2.21	0.41
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.55	0.41
1:A:436:LYS:HG2	1:A:437:VAL:N	2.36	0.41
1:A:521:VAL:CG2	1:A:522:ILE:N	2.82	0.41
1:A:540:PRO:C	1:A:542:LYS:N	2.78	0.41
1:A:744:VAL:O	1:A:745:ALA:C	2.63	0.41
1:A:181:THR:HG22	1:A:706:ASN:ND2	2.36	0.41
1:A:778:THR:HG22	1:A:779:ALA:N	2.35	0.41
1:A:947:ILE:HB	1:A:957:PHE:HE1	1.85	0.41
1:A:962:LEU:O	1:A:963:ASP:C	2.63	0.41
1:A:965:THR:O	1:A:969:MET:HB2	2.21	0.41
1:A:48:SER:O	1:A:52:LEU:HG	2.21	0.41
1:A:200:VAL:HG21	1:A:489:ARG:NH2	2.27	0.41
1:A:82:GLU:CD	1:A:82:GLU:N	2.79	0.41
1:A:180:LEU:HD23	1:A:705:VAL:HG11	2.02	0.41
1:A:242:THR:HG23	1:A:712:LYS:HZ2	1.85	0.41
1:A:289:ILE:O	1:A:289:ILE:HG22	2.21	0.41
1:A:408:ASP:O	1:A:410:LEU:N	2.54	0.41
1:A:444:ALA:HB3	1:A:599:MET:HE1	2.02	0.41
1:A:495:SER:HA	1:A:513:PHE:O	2.20	0.41
1:A:512:MET:O	1:A:566:THR:HA	2.20	0.41
1:A:572:LYS:O	1:A:573:ARG:C	2.63	0.41
1:A:669:ALA:O	1:A:673:ALA:HB2	2.21	0.41
1:A:751:ARG:NH2	1:A:821:PRO:CA	2.84	0.41
1:A:920:GLN:OE1	1:A:924:ARG:HD3	2.21	0.41
1:A:10:GLU:OE1	1:A:10:GLU:N	2.51	0.41
1:A:107:TRP:CD1	1:A:111:ASN:HD21	2.37	0.41
1:A:558:THR:OG1	1:A:638:ARG:NH1	2.53	0.41
1:A:576:MET:HE3	1:A:587:TYR:HB3	2.03	0.41
1:A:52:LEU:O	1:A:55:GLU:N	2.54	0.40
1:A:764:LEU:HD21	1:A:804:ALA:HB2	2.04	0.40
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.39	0.40
1:A:683:HIS:O	1:A:684:LYS:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:TRP:C	1:A:856:PHE:N	2.77	0.40
1:A:290:ARG:HG2	1:A:290:ARG:O	2.21	0.40
1:A:311:LEU:HB3	1:A:312:PRO:HD3	2.03	0.40
1:A:367:PHE:C	1:A:367:PHE:HD1	2.29	0.40
1:A:473:SER:HA	1:A:476:ARG:HD2	2.03	0.40
1:A:791:GLN:O	1:A:792:LEU:C	2.64	0.40
1:A:869:GLN:C	1:A:871:THR:N	2.75	0.40
1:A:58:GLU:O	1:A:63:ARG:NH1	2.55	0.40
1:A:667:ARG:NH1	1:A:694:TYR:CZ	2.89	0.40
1:A:882:HIS:ND1	1:A:882:HIS:C	2.80	0.40
1:A:18:VAL:HG23	1:A:24:LEU:HD12	2.02	0.40
1:A:532:THR:C	1:A:533:THR:HG22	2.46	0.40
1:A:540:PRO:O	1:A:542:LYS:N	2.54	0.40
1:A:628:ASN:O	1:A:629:LYS:C	2.63	0.40
1:A:650:ASP:O	1:A:672:ARG:HD2	2.22	0.40
1:A:767:SER:O	1:A:768:ASN:C	2.64	0.40
1:A:962:LEU:O	1:A:966:GLN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	992/994 (100%)	811 (82%)	146 (15%)	35 (4%)	3 16

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	VAL
1	A	531	GLY
1	A	581	SER
1	A	681	PRO

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Mol	Chain	Res	Type
1	A	683	HIS
1	A	889	GLU
1	A	78	PHE
1	A	110	ARG
1	A	227	GLY
1	A	432	GLY
1	A	507	ALA
1	A	663	LEU
1	A	677	ALA
1	A	738	ASP
1	A	905	VAL
1	A	957	PHE
1	A	963	ASP
1	A	991	TYR
1	A	47	LYS
1	A	453	ASN
1	A	502	LYS
1	A	649	ALA
1	A	793	LEU
1	A	882	HIS
1	A	42	PRO
1	A	975	LEU
1	A	540	PRO
1	A	956	ILE
1	A	541	VAL
1	A	951	ASP
1	A	409	GLY
1	A	53	VAL
1	A	195	PRO
1	A	783	LEU
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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	840/840 (100%)	778 (93%)	62 (7%)	13 40

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	19	SER
1	A	26	PRO
1	A	82	GLU
1	A	117	GLU
1	A	146	VAL
1	A	160	PRO
1	A	175	VAL
1	A	187	VAL
1	A	191	THR
1	A	208	LEU
1	A	226	THR
1	A	228	VAL
1	A	247	THR
1	A	340	GLU
1	A	344	CYS
1	A	353	THR
1	A	358	THR
1	A	367	PHE
1	A	368	ILE
1	A	396	LEU
1	A	446	THR
1	A	449	VAL
1	A	457	THR
1	A	474	VAL
1	A	484	THR
1	A	494	MET
1	A	512	MET
1	A	514	VAL
1	A	521	VAL
1	A	533	THR
1	A	537	MET
1	A	541	VAL
1	A	569	THR
1	A	577	VAL

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Mol	Chain	Res	Type
1	A	594	VAL
1	A	596	VAL
1	A	597	VAL
1	A	606	GLU
1	A	628	ASN
1	A	638	ARG
1	A	681	PRO
1	A	698	THR
1	A	703	ASP
1	A	716	ILE
1	A	760	PHE
1	A	765	ILE
1	A	778	THR
1	A	805	THR
1	A	811	PRO
1	A	816	ILE
1	A	844	VAL
1	A	867	TYR
1	A	870	LEU
1	A	878	GLU
1	A	895	GLU
1	A	898	THR
1	A	910	CYS
1	A	925	MET
1	A	940	SER
1	A	957	PHE
1	A	963	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	111	ASN
1	A	138	GLN
1	A	177	GLN
1	A	259	GLN
1	A	278	HIS
1	A	380	ASN
1	A	398	ASN
1	A	453	ASN
1	A	472	ASN
1	A	526	ASN

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Mol	Chain	Res	Type
1	A	628	ASN
1	A	666	GLN
1	A	683	HIS
1	A	692	GLN
1	A	706	ASN
1	A	759	GLN
1	A	796	ASN
1	A	869	GLN
1	A	875	GLN
1	A	914	ASN
1	A	944	HIS
1	A	990	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	-	44,48,48	1.93	12 (27%)	47,72,72	1.94	10 (21%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1995	TG1	O4-C21	5.72	1.33	1.21
2	A	1995	TG1	O3-C3	4.26	1.52	1.44
2	A	1995	TG1	O6-C7	4.22	1.50	1.43
2	A	1995	TG1	O1-C13	3.71	1.44	1.34
2	A	1995	TG1	C34-C11	3.36	1.57	1.53
2	A	1995	TG1	O11-C11	2.74	1.47	1.42
2	A	1995	TG1	C21-C22	2.73	1.58	1.50
2	A	1995	TG1	O7-C27	2.69	1.41	1.34
2	A	1995	TG1	C31-C10	2.39	1.57	1.52
2	A	1995	TG1	C1-C2	2.36	1.58	1.54
2	A	1995	TG1	C11-C7	2.22	1.58	1.55
2	A	1995	TG1	C9-C10	2.10	1.57	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1995	TG1	C10-O9-C32	6.97	137.68	121.36
2	A	1995	TG1	C24-C22-C21	3.50	133.92	120.79
2	A	1995	TG1	C7-C6-C5	3.44	124.44	115.41
2	A	1995	TG1	O12-C12-C11	-3.32	124.92	128.28
2	A	1995	TG1	O5-C12-O12	3.20	125.74	121.60
2	A	1995	TG1	C6-O5-C12	-3.19	106.37	110.80
2	A	1995	TG1	C23-C22-C21	-2.84	108.81	116.12
2	A	1995	TG1	C2-O1-C13	-2.65	113.29	117.59
2	A	1995	TG1	O1-C2-C3	-2.29	105.86	110.18
2	A	1995	TG1	O7-C27-O8	2.10	128.62	123.70

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1995	TG1	C33-C32-O9-C10

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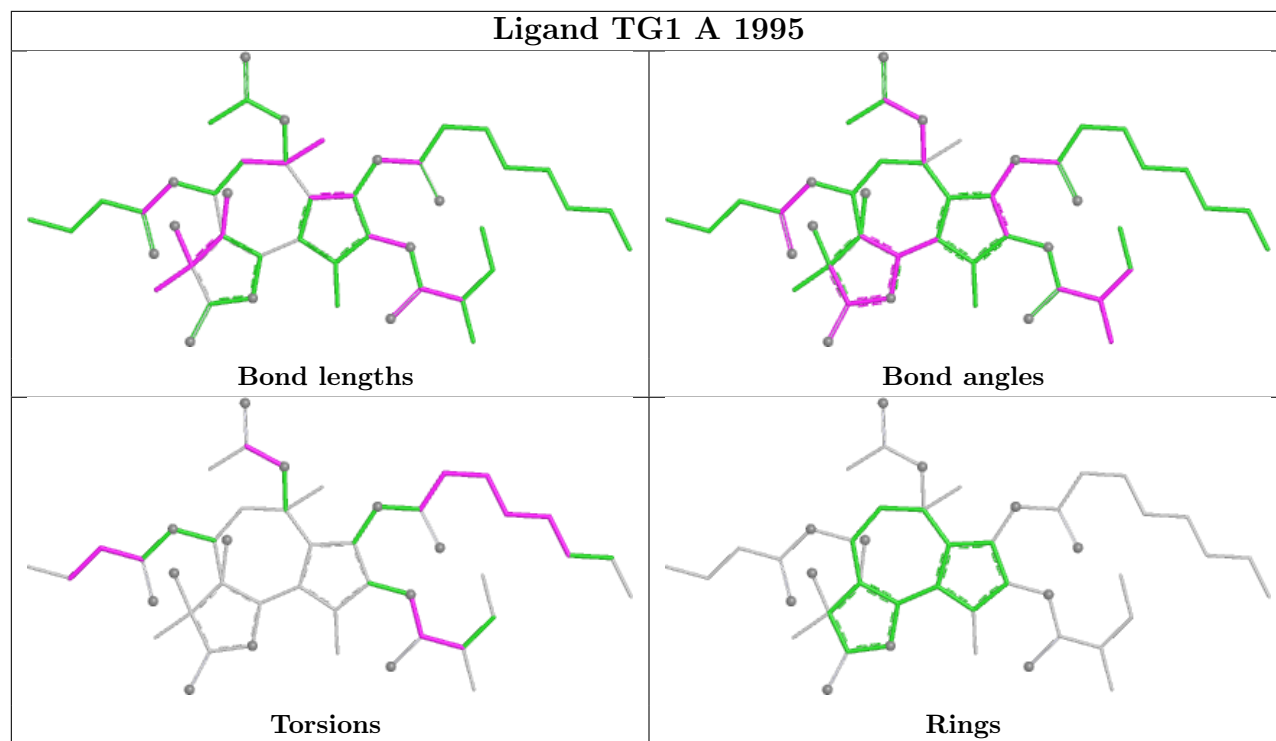
Mol	Chain	Res	Type	Atoms
2	A	1995	TG1	O4-C21-C22-C24
2	A	1995	TG1	O10-C32-O9-C10
2	A	1995	TG1	O4-C21-C22-C23
2	A	1995	TG1	C15-C16-C17-C18
2	A	1995	TG1	C27-C28-C29-C30
2	A	1995	TG1	O3-C21-C22-C23
2	A	1995	TG1	C16-C17-C18-C19
2	A	1995	TG1	C13-C14-C15-C16
2	A	1995	TG1	O3-C21-C22-C24
2	A	1995	TG1	C14-C15-C16-C17
2	A	1995	TG1	O1-C13-C14-C15
2	A	1995	TG1	C22-C21-O3-C3
2	A	1995	TG1	O7-C27-C28-C29
2	A	1995	TG1	O2-C13-C14-C15
2	A	1995	TG1	O8-C27-C28-C29

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1995	TG1	5	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.23	17 (1%) 69 48	19, 62, 136, 184	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	862	GLY	3.1
1	A	280	ASN	3.0
1	A	959	LEU	2.8
1	A	974	SER	2.6
1	A	958	LYS	2.6
1	A	1	MET	2.5
1	A	879	ASP	2.5
1	A	866	THR	2.4
1	A	965	THR	2.4
1	A	877	THR	2.3
1	A	888	CYS	2.3
1	A	880	HIS	2.2
1	A	281	ASP	2.1
1	A	289	ILE	2.1
1	A	884	GLU	2.1
1	A	581	SER	2.0
1	A	284	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

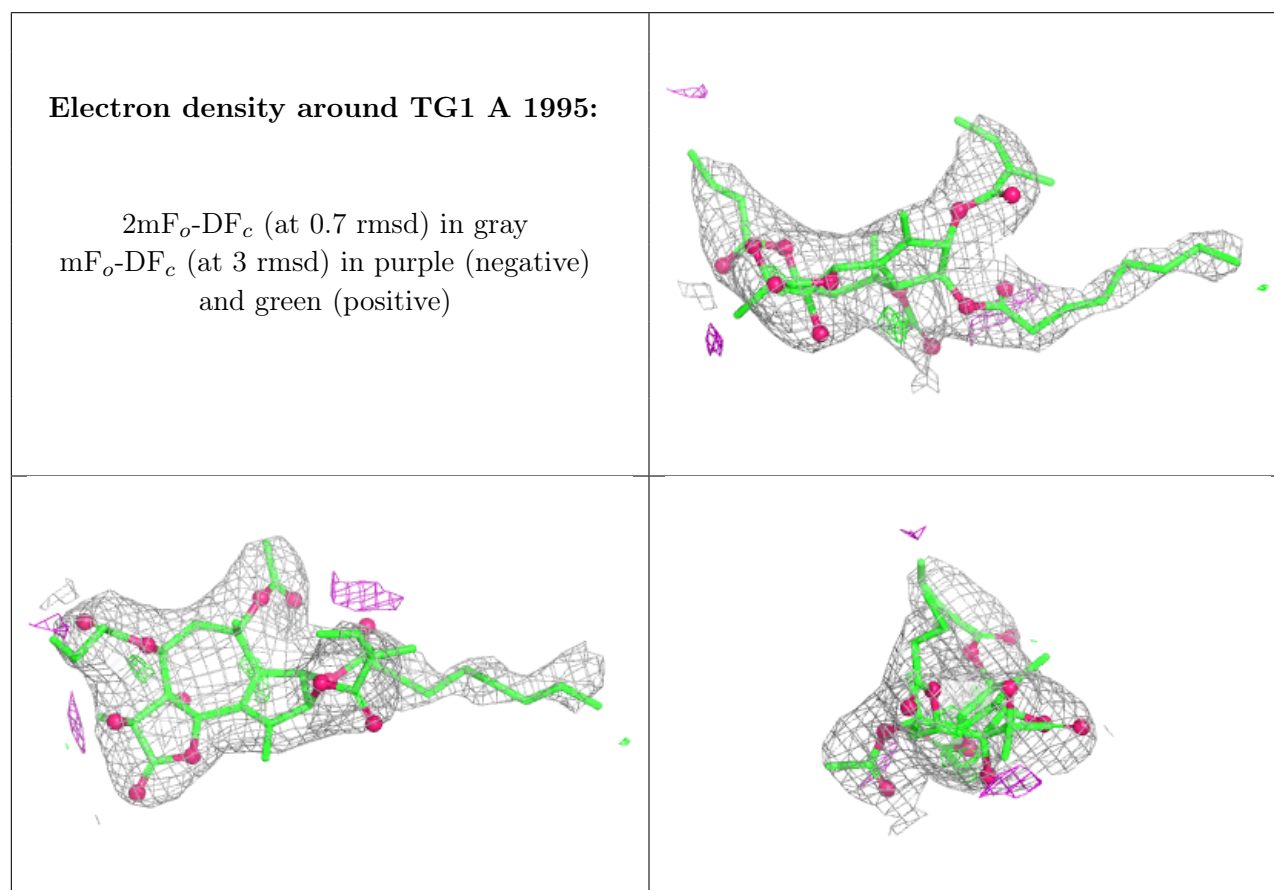
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	1996	1/1	0.90	0.17	52,52,52,52	0
2	TG1	A	1995	46/46	0.91	0.11	55,59,60,61	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.