



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:51 pm BST

PDB ID : 4J2T  
Title : Inhibitor-bound Ca<sup>2+</sup> ATPase  
Authors : Paulsen, E.S.; Villadsen, J.; Tenori, E.; Liu, H.; Lie, M.A.; Bonde, D.F.;  
Bublitz, M.; Olesen, C.; Autzen, H.E.; Dach, I.; Sehgal, P.; Moller, J.V.;  
Schlott, B.; Nissen, P.; Christensen, S.B.  
Deposited on : 2013-02-05  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

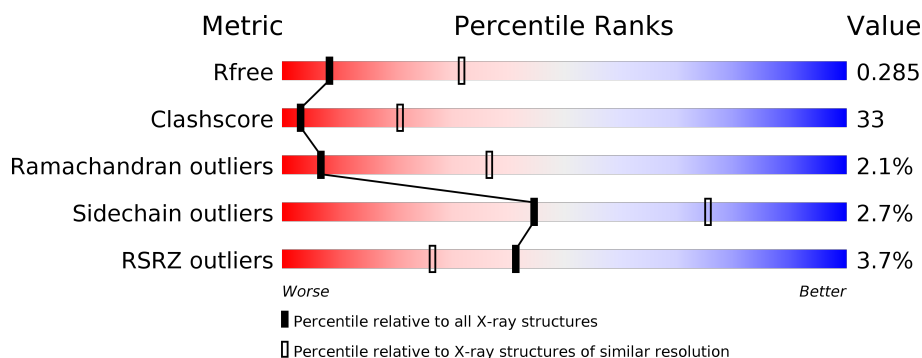
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	994	<div> <div>4%</div> <div>49%</div> <div>48%</div> <div>.</div> </div>

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	PTY	A	1002	-	-	-	X

## 2 Entry composition [i](#)

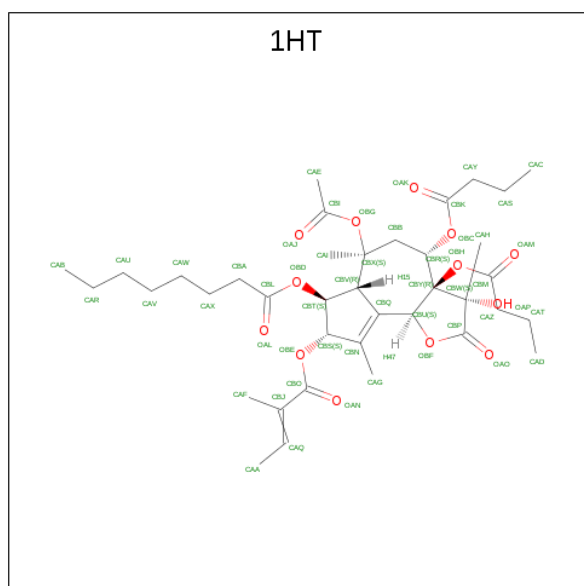
There are 5 unique types of molecules in this entry. The entry contains 7748 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERCA1a.

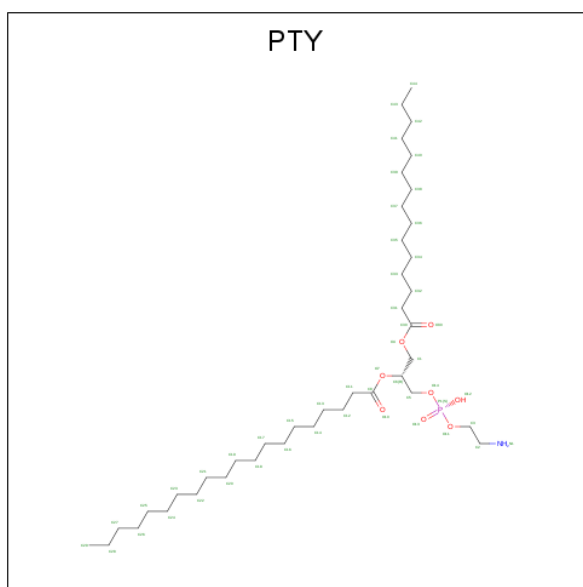
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	994	7671	4876	1287	1451	57	0	0	0

- Molecule 2 is (3S,3aR,4S,6S,6aR,7S,8S,9bS)-6-(acetyloxy)-3a,4-bis(butanoyloxy)-3-hydroxy-3,6,9-trimethyl-8-{[(2E)-2-methylbut-2-enoyl]oxy}-2-oxo-2,3,3a,4,5,6,6a,7,8,9b-decahydroazuleno[4,5-b]furan-7-yl octanoate (three-letter code: 1HT) (formula: C<sub>38</sub>H<sub>56</sub>O<sub>13</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	51	38	13	0	0

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	14	1	8	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

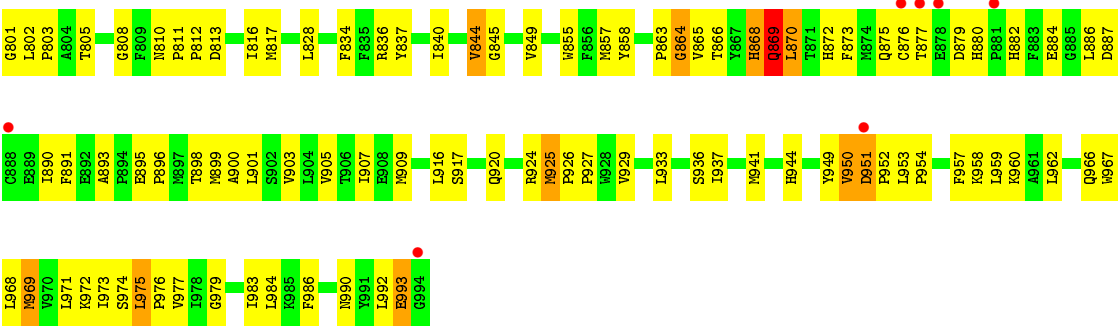
- Molecule 5 is water.

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

Chain A: 

Node	Parent	Value	Color	Category				
M1	T86	Q177	T1267	T345	C417	R560	F642	V726
S6	A87	S178	A270	C349	C420	L564	G643	S731
T9	F88	L180	V271	T282	N421	R489	G643	E732
E10	B90	T181	T272	K352	D422	R491	E646	M733
E10	P91	G182	L273	T353	S423	S495	E647	M737
L13	L95	E183	I274	G354	V496	D568	V648	D737
A14	L96	V187	N280	T355	L425	R573	T854	M739
A14	L97	I188	D281	T357	N428	E574	G655	M739
G17	L98	K189	P282	T358	E429	E575	G656	F740
V18	I99	E192	T283	N359	T430	N576	R656	S741
S19	A100	V194	I284	Q360	V433	R502	E657	S741
T22	M101	G285	G286	M361	Y434	P500	T855	A746
G23	A102	I103	S287	S362	Y434	E501	E656	E747
L24	I104	V104	H288	V363	E435	D579	G657	F747
T25	G105	G105	L289	C364	A506	S504	S581	E749
Q28	V106	Q202	R290	K365	K436	R505	S582	G750
Q28	Q107	D203	G291	P366	V437	E507	R583	R751
R31	Q108	K205	D203	T367	T441	N508	E666	A752
H32	E109	K206	N206	D370	E442	G509	E667	F752
N39	M114	H207	Y294	K371	T445	E519	E668	E753
E40	E117	L208	K297	D375	T446	T446	E585	F753
E44	E122	I214	I298	F376	T447	E520	E586	E754
E44	Y122	A219	A299	G377	L448	N521	E587	F754
G46	K128	L220	A301	L379	V449	E522	E588	E755
K47	V129	G221	A303	N380	E451	N523	E675	M760
S48	V130	I222	A303	F381	K452	R524	E676	I761
L49	R131	V223	A305	F382	V450	E527	E677	L764
W50	A132	A224	A306	F455	E455	V528	E678	E765
E51	T225	T225	I307	S383	N456	R529	E679	S767
L52	K135	T226	L307	I384	T457	V530	E680	M769
V53	S136	I235	L311	Y389	E458	E607	E683	V769
I54	V137	I235	P312	A390	V459	R533	E684	G770
D59	R143	M239	A313	E392	R460	H534	E688	E771
L60	V146	T242	V314	E393	N461	M608	E688	V772
L61	P147	E243	I315	G393	L462	Q612	L691	C774
V62	G148	Q244	T317	E394	E466	R615	Q692	L777
R63	D149	Q244	C318	V395	R467	D616	S693	E777
L65	I150	T247	L319	K397	E470	P540	V694	L781
C70	V151	P248	A320	P401	C471	V541	D695	G783
I71	E152	L249	L321	I402	N472	K542	I622	L783
L75	V159	Q250	M326	R403	S473	T545	D627	I788
A76	P160	L253	K329	S404	I475	E549	N628	P789
F77	I163	E258	L336	F407	R476	K550	G629	V790
F78	Q259	L260	P337	G409	L478	E552	E630	G791
E79	S261	L166	S338	L410	N479	G553	T631	V705
E80	L166	E262	V339	V411	E482	T654	A632	L793
G81	L173	V263	E340	E412	F483	E555	I633	P709
E82	R174	I264	T341	E412	T484	R556	A634	E709
E83	E174	L264	L342	T415	L495	D657	E636	V795
E83	E174	L264	L342	T415	L495	T550	R637	F795
E83	E174	L264	L342	T415	L495	T550	E638	M720
E83	E174	L264	L342	T41				



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.90 Å 70.90 Å 587.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.71 – 3.20 28.71 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.71-3.20) 99.6 (28.71-3.01)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 3.00 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.260 , 0.286 0.261 , 0.285	Depositor DCC
$R_{free}$ test set	2000 reflections (6.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.5	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 55.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7748	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: K, PTY, 1HT

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	0.46	1/7812 (0.0%)	0.69	1/10592 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	ASN	C-N	-5.05	1.22	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	870	LEU	N-CA-C	-5.64	95.78	111.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7671	0	7764	515	0
2	A	51	0	55	8	0
3	A	24	0	21	4	0
4	A	1	0	0	0	0
5	A	1	0	0	2	0
All	All	7748	0	7840	515	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 33.

All (515) 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:527:TYR:HB2	1:A:592:THR:CG2	1.45	1.45
1:A:527:TYR:CB	1:A:592:THR:HG22	1.40	1.45
1:A:483:PHE:CE1	1:A:578:LEU:HD21	1.73	1.22
1:A:534:ARG:HD2	1:A:592:THR:HG21	1.40	1.02
1:A:834:PHE:HE2	2:A:1001:1HT:OAM	1.43	1.01
1:A:425:LEU:HD11	1:A:447:THR:HG22	1.44	0.99
1:A:863:PRO:HG3	1:A:890:ILE:HD13	1.42	0.99
1:A:247:THR:HG22	1:A:250:GLN:H	1.24	0.98
1:A:483:PHE:CE1	1:A:578:LEU:CD2	2.48	0.96
1:A:311:LEU:HD13	1:A:764:LEU:HD12	1.49	0.94
1:A:909:MET:HE3	1:A:937:ILE:HG12	1.47	0.94
1:A:97:ILE:HD11	1:A:797:LEU:HD11	1.50	0.94
1:A:32:HIS:HB3	1:A:146:VAL:HG11	1.48	0.93
1:A:483:PHE:CZ	1:A:578:LEU:HD21	2.02	0.93
1:A:558:THR:HG22	1:A:634:ALA:HB1	1.51	0.93
1:A:304:VAL:HB	1:A:793:LEU:HD21	1.48	0.93
1:A:65:LEU:HG	1:A:307:ILE:CD1	2.00	0.90
1:A:248:PRO:HG2	1:A:340:GLU:OE2	1.73	0.89
1:A:654:THR:HG22	1:A:657:GLU:HG3	1.54	0.89
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.56	0.87
1:A:880:HIS:HA	1:A:884:GLU:HB2	1.57	0.87
1:A:535:VAL:HG13	1:A:536:PRO:HD2	1.55	0.86
1:A:1:MET:HB2	1:A:225:THR:HG22	1.57	0.86
1:A:527:TYR:CG	1:A:592:THR:HG22	2.11	0.84
1:A:361:MET:HE3	1:A:599:MET:HG3	1.59	0.83
1:A:1:MET:HA	1:A:224:ALA:O	1.79	0.83
1:A:75:LEU:HD13	1:A:297:LYS:HB3	1.60	0.82
1:A:834:PHE:CE2	2:A:1001:1HT:OAM	2.31	0.82
1:A:879:ASP:OD1	1:A:882:HIS:HB3	1.80	0.81
1:A:453:ASN:HB3	1:A:471:CYS:SG	2.21	0.81
1:A:558:THR:HG22	1:A:634:ALA:CB	2.12	0.80
1:A:47:LYS:HA	1:A:51:GLU:OE1	1.81	0.80
1:A:628:ASN:HB3	1:A:678:ARG:NH2	1.95	0.80
1:A:986:PHE:CZ	1:A:990:ASN:OD1	2.34	0.80
1:A:788:ILE:HG23	1:A:789:PRO:HD2	1.64	0.80
1:A:287:SER:HB2	1:A:290:ARG:HB3	1.63	0.79
1:A:986:PHE:CE1	1:A:990:ASN:OD1	2.36	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:O	1:A:274:ILE:HG12	1.82	0.79
1:A:396:LEU:HD23	1:A:401:PRO:HA	1.64	0.78
1:A:907:ILE:HG23	1:A:977:VAL:HG21	1.65	0.78
1:A:857:MET:O	1:A:858:TYR:HB2	1.83	0.78
1:A:65:LEU:HG	1:A:307:ILE:HD12	1.65	0.78
1:A:267:ILE:HD11	2:A:1001:1HT:H2	1.65	0.77
1:A:32:HIS:HB3	1:A:146:VAL:CG1	2.14	0.76
1:A:106:VAL:C	1:A:108:GLN:H	1.88	0.76
1:A:239:MET:O	1:A:242:THR:HG22	1.85	0.76
1:A:32:HIS:CB	1:A:146:VAL:HG11	2.16	0.76
1:A:549:ILE:HD11	1:A:596:VAL:HG11	1.66	0.76
1:A:342:LEU:O	1:A:345:THR:HG23	1.86	0.74
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.69	0.74
1:A:628:ASN:HB3	1:A:678:ARG:HH21	1.52	0.74
1:A:247:THR:HG22	1:A:250:GLN:N	2.01	0.74
1:A:748:GLU:HA	1:A:817:MET:HE3	1.68	0.73
1:A:769:VAL:HG22	2:A:1001:1HT:H58	1.68	0.73
1:A:865:VAL:HG23	1:A:868:HIS:NE2	2.02	0.73
1:A:522:ILE:HG22	1:A:542:LYS:HE3	1.71	0.73
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.71	0.72
1:A:751:ARG:HD2	1:A:817:MET:CE	2.19	0.72
1:A:106:VAL:C	1:A:108:GLN:N	2.41	0.72
1:A:969:MET:HA	1:A:969:MET:HE3	1.72	0.72
1:A:751:ARG:HD2	1:A:817:MET:HE2	1.72	0.71
1:A:153:VAL:HB	1:A:214:ILE:CD1	2.20	0.71
1:A:654:THR:HG22	1:A:657:GLU:CG	2.19	0.71
1:A:748:GLU:HG3	1:A:817:MET:HE3	1.71	0.71
1:A:717:GLY:O	1:A:731:SER:HB2	1.91	0.71
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.73	0.71
1:A:65:LEU:HG	1:A:307:ILE:HD13	1.74	0.70
1:A:441:THR:HG21	1:A:560:ARG:NH1	2.07	0.70
1:A:535:VAL:CG1	1:A:536:PRO:HD2	2.20	0.69
1:A:870:LEU:O	1:A:873:PHE:HB3	1.92	0.69
1:A:361:MET:HE2	1:A:441:THR:HG22	1.75	0.69
1:A:436:LYS:HG3	1:A:443:THR:HG21	1.75	0.68
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.75	0.68
1:A:813:ASP:O	1:A:816:ILE:HG13	1.93	0.68
1:A:971:LEU:HD22	1:A:975:LEU:HD11	1.74	0.68
1:A:969:MET:O	1:A:973:ILE:HG13	1.93	0.68
1:A:97:ILE:CD1	1:A:797:LEU:HD11	2.21	0.68
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.29	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:PHE:HB2	1:A:457:THR:HG23	1.74	0.68
1:A:530:VAL:HG23	1:A:533:THR:OG1	1.95	0.67
1:A:79:GLU:HG3	1:A:87:ALA:CB	2.25	0.67
1:A:192:GLU:OE1	1:A:580:ASP:HB2	1.95	0.67
1:A:411:VAL:O	1:A:415:THR:HG23	1.94	0.67
1:A:791:GLN:HB3	1:A:901:LEU:CD1	2.24	0.67
1:A:909:MET:CE	1:A:937:ILE:HA	2.25	0.67
1:A:179:ILE:HG13	1:A:180:LEU:N	2.09	0.66
1:A:837:TYR:HB2	2:A:1001:IHT:H16	1.77	0.66
1:A:757:MET:HA	1:A:760:PHE:CE2	2.30	0.66
1:A:791:GLN:HB3	1:A:901:LEU:HD12	1.77	0.66
1:A:541:VAL:O	1:A:545:ILE:HG13	1.96	0.65
1:A:781:LEU:HB2	1:A:783:LEU:HD13	1.77	0.65
1:A:903:VAL:O	1:A:907:ILE:HG13	1.96	0.65
1:A:235:ILE:HG23	1:A:709:PRO:HG3	1.78	0.65
1:A:553:GLY:O	1:A:631:THR:HG22	1.96	0.65
1:A:857:MET:HA	1:A:864:GLY:HA2	1.79	0.65
1:A:863:PRO:CG	1:A:890:ILE:HD13	2.22	0.65
1:A:368:ILE:HD13	1:A:410:LEU:HD23	1.77	0.65
1:A:146:VAL:HG13	1:A:147:PRO:HD2	1.79	0.65
1:A:397:LYS:HB3	1:A:402:ILE:HD11	1.78	0.65
1:A:105:GLY:O	1:A:108:GLN:HB3	1.96	0.65
1:A:247:THR:HG23	1:A:340:GLU:OE1	1.96	0.65
1:A:44:GLU:H	1:A:44:GLU:CD	1.99	0.64
1:A:527:TYR:CD2	1:A:592:THR:CG2	2.80	0.64
1:A:951:ASP:O	1:A:954:PRO:HD2	1.96	0.64
1:A:99:ILE:O	1:A:103:ILE:HG12	1.97	0.64
1:A:153:VAL:HB	1:A:214:ILE:HD11	1.78	0.64
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.27	0.64
1:A:606:GLU:CD	1:A:606:GLU:H	2.00	0.64
1:A:527:TYR:CB	1:A:592:THR:CG2	2.30	0.64
1:A:527:TYR:HB2	1:A:592:THR:CB	2.23	0.64
1:A:49:LEU:O	1:A:53:VAL:HG23	1.98	0.64
1:A:282:PRO:HB2	1:A:284:HIS:NE2	2.13	0.64
1:A:484:THR:HG22	1:A:496:VAL:HG12	1.80	0.64
1:A:304:VAL:HB	1:A:793:LEU:CD2	2.24	0.64
1:A:654:THR:CG2	1:A:657:GLU:HG3	2.25	0.64
1:A:9:THR:HG23	1:A:166:LEU:HD22	1.79	0.63
1:A:420:CYS:SG	1:A:515:LYS:HG2	2.39	0.63
1:A:527:TYR:CD2	1:A:592:THR:HG22	2.33	0.63
1:A:192:GLU:OE1	1:A:580:ASP:CB	2.47	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HB2	1:A:83:GLU:OE1	1.97	0.63
1:A:18:VAL:CG2	1:A:24:LEU:HD23	2.29	0.63
1:A:662:PRO:HG2	1:A:665:GLU:OE1	1.98	0.63
1:A:317:THR:O	1:A:321:LEU:HG	1.99	0.63
1:A:244:GLN:HB3	5:A:1101:HOH:O	1.98	0.62
1:A:869:GLN:CB	1:A:872:HIS:ND1	2.62	0.62
1:A:483:PHE:CD1	1:A:578:LEU:CD2	2.82	0.62
1:A:508:VAL:HG23	1:A:508:VAL:O	2.00	0.62
1:A:263:VAL:HG11	2:A:1001:1HT:OAN	2.00	0.62
1:A:65:LEU:CG	1:A:307:ILE:HD12	2.30	0.62
1:A:577:VAL:HG21	1:A:583:ARG:NH1	2.15	0.61
1:A:907:ILE:HG12	1:A:974:SER:CB	2.30	0.61
1:A:962:LEU:HD12	1:A:967:TRP:CD1	2.35	0.61
1:A:6:SER:HA	1:A:194:VAL:O	2.01	0.61
1:A:629:LYS:HA	1:A:632:ALA:HB3	1.83	0.61
1:A:358:THR:HG22	1:A:360:GLN:HG3	1.82	0.61
1:A:59:ASP:O	1:A:62:VAL:HG12	2.01	0.61
1:A:671:ARG:HD2	1:A:694:TYR:CE1	2.36	0.61
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.36	0.61
1:A:203:ASP:HA	1:A:205:LYS:HE3	1.81	0.61
1:A:45:GLU:OE2	1:A:47:LYS:HG3	2.00	0.61
1:A:870:LEU:HD12	1:A:891:PHE:HE1	1.66	0.61
1:A:483:PHE:CD2	1:A:578:LEU:HD11	2.36	0.60
1:A:900:ALA:HA	1:A:903:VAL:HG12	1.82	0.60
1:A:22:THR:HG23	1:A:132:ALA:HB2	1.83	0.60
1:A:748:GLU:HA	1:A:817:MET:CE	2.31	0.60
1:A:865:VAL:HG23	1:A:868:HIS:CD2	2.36	0.60
1:A:545:ILE:O	1:A:549:ILE:HG12	2.02	0.60
1:A:367:PHE:CD1	1:A:379:LEU:HD23	2.37	0.60
1:A:836:ARG:O	1:A:840:ILE:HG12	2.00	0.60
1:A:500:PRO:O	1:A:501:ALA:HB3	2.02	0.60
1:A:900:ALA:O	1:A:903:VAL:HG12	2.02	0.60
1:A:24:LEU:HG	1:A:149:ASP:HA	1.83	0.59
1:A:65:LEU:CD2	1:A:307:ILE:HD12	2.32	0.59
1:A:876:CYS:SG	1:A:884:GLU:HG2	2.42	0.59
1:A:636:CYS:HB3	1:A:642:PHE:CD2	2.37	0.59
1:A:9:THR:HG23	1:A:166:LEU:CD2	2.33	0.58
1:A:415:THR:HA	1:A:475:ILE:HD13	1.86	0.58
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.32	0.58
1:A:193:PRO:HA	1:A:206:ASN:ND2	2.18	0.58
1:A:473:SER:HA	1:A:476:ARG:HD2	1.84	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:THR:HA	1:A:599:MET:HE2	1.84	0.58
1:A:895:GLU:N	1:A:896:PRO:HD2	2.17	0.58
1:A:557:ASP:HB3	1:A:559:LEU:HG	1.84	0.58
1:A:507:ALA:O	1:A:508:VAL:HG22	2.04	0.58
1:A:355:THR:HG21	1:A:720:MET:CE	2.33	0.58
1:A:61:LEU:HD21	1:A:260:LEU:HD23	1.85	0.58
1:A:688:VAL:O	1:A:692:GLN:HG3	2.03	0.58
1:A:363:VAL:HA	1:A:599:MET:HA	1.85	0.58
1:A:840:ILE:O	1:A:844:VAL:HG13	2.03	0.58
1:A:473:SER:HA	1:A:476:ARG:HB2	1.84	0.57
1:A:539:GLY:N	1:A:540:PRO:HD2	2.18	0.57
1:A:71:ILE:HB	1:A:300:VAL:CG1	2.35	0.57
1:A:367:PHE:HZ	1:A:545:ILE:HG23	1.69	0.57
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.85	0.57
1:A:397:LYS:CB	1:A:402:ILE:HD11	2.34	0.57
1:A:369:ILE:HD13	1:A:528:VAL:HB	1.86	0.57
1:A:917:SER:OG	1:A:920:GLN:HB2	2.04	0.57
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.87	0.57
1:A:326:MET:O	1:A:329:LYS:N	2.37	0.57
1:A:301:ALA:HA	1:A:789:PRO:HG3	1.87	0.57
1:A:869:GLN:HB2	1:A:872:HIS:ND1	2.20	0.57
1:A:441:THR:HA	1:A:599:MET:CE	2.35	0.56
1:A:10:GLU:N	1:A:10:GLU:OE1	2.38	0.56
1:A:654:THR:HG23	1:A:656:ARG:H	1.69	0.56
1:A:79:GLU:HG3	1:A:87:ALA:HB1	1.86	0.56
1:A:444:ALA:HB3	1:A:599:MET:HE1	1.88	0.56
1:A:79:GLU:HG3	1:A:87:ALA:HB2	1.88	0.56
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.87	0.56
1:A:483:PHE:CD1	1:A:578:LEU:HD22	2.40	0.56
1:A:61:LEU:CD2	1:A:260:LEU:HD23	2.36	0.56
1:A:617:ALA:HB1	1:A:751:ARG:HH12	1.69	0.56
1:A:875:GLN:O	1:A:875:GLN:HG3	2.06	0.56
1:A:363:VAL:CG1	1:A:597:VAL:HG13	2.35	0.56
1:A:189:LYS:HD2	1:A:205:LYS:O	2.06	0.56
1:A:863:PRO:HG3	1:A:890:ILE:HG21	1.87	0.56
1:A:104:VAL:O	1:A:108:GLN:HB2	2.06	0.56
1:A:177:GLN:O	1:A:178:SER:C	2.44	0.56
1:A:383:SER:C	1:A:384:ILE:HD12	2.25	0.56
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.41	0.56
1:A:411:VAL:CB	1:A:454:VAL:HG11	2.36	0.55
1:A:411:VAL:HG12	1:A:454:VAL:CG1	2.35	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:CG2	1:A:250:GLN:HG3	2.36	0.55
1:A:979:GLY:O	1:A:983:ILE:HG13	2.06	0.55
1:A:648:VAL:O	1:A:648:VAL:HG12	2.06	0.55
1:A:367:PHE:CD2	1:A:596:VAL:HG22	2.41	0.55
1:A:788:ILE:HG23	1:A:789:PRO:CD	2.36	0.55
1:A:470:ALA:O	1:A:474:VAL:HG23	2.06	0.55
1:A:247:THR:HB	1:A:250:GLN:HG3	1.88	0.55
1:A:369:ILE:CD1	1:A:528:VAL:HB	2.37	0.55
1:A:128:LYS:O	1:A:151:VAL:HG13	2.06	0.55
1:A:381:GLU:O	1:A:397:LYS:HD2	2.07	0.55
1:A:264:ILE:HG23	1:A:302:LEU:HD21	1.89	0.54
1:A:313:ALA:O	1:A:317:THR:HG23	2.07	0.54
1:A:408:ASP:O	1:A:411:VAL:HG22	2.06	0.54
1:A:436:LYS:CG	1:A:443:THR:HG21	2.36	0.54
1:A:122:TYR:HE2	1:A:726:VAL:CG2	2.19	0.54
1:A:394:GLU:HG3	1:A:396:LEU:HD21	1.88	0.54
1:A:411:VAL:HA	1:A:454:VAL:HG21	1.89	0.54
1:A:801:GLY:O	1:A:805:THR:HG23	2.07	0.54
1:A:179:ILE:O	1:A:705:VAL:HG12	2.08	0.54
1:A:100:ALA:HB3	3:A:1002:PTY:H311	1.89	0.54
1:A:553:GLY:CA	1:A:631:THR:HG22	2.38	0.54
1:A:880:HIS:HA	1:A:884:GLU:CB	2.36	0.54
1:A:358:THR:O	1:A:359:ASN:HB3	2.08	0.54
1:A:575:GLU:OE1	1:A:575:GLU:HA	2.08	0.54
1:A:247:THR:HG23	1:A:249:LEU:H	1.73	0.54
1:A:519:GLU:H	1:A:519:GLU:CD	2.11	0.53
1:A:384:ILE:HD12	1:A:384:ILE:N	2.23	0.53
1:A:391:PRO:HD2	1:A:434:TYR:CE2	2.43	0.53
1:A:654:THR:CG2	1:A:657:GLU:H	2.20	0.53
1:A:22:THR:HG22	1:A:23:GLY:O	2.08	0.53
1:A:433:VAL:HG12	1:A:434:TYR:N	2.24	0.53
1:A:857:MET:O	1:A:858:TYR:CB	2.55	0.53
1:A:75:LEU:CD1	1:A:297:LYS:HB3	2.36	0.53
1:A:86:THR:O	1:A:89:VAL:HG22	2.08	0.53
1:A:497:TYR:CD2	1:A:512:MET:HE3	2.44	0.53
1:A:363:VAL:HG11	1:A:597:VAL:HG13	1.90	0.53
1:A:363:VAL:HG22	1:A:599:MET:HB3	1.89	0.53
1:A:777:LEU:HB2	1:A:849:VAL:HG21	1.89	0.53
1:A:757:MET:HG3	1:A:760:PHE:CZ	2.44	0.52
1:A:920:GLN:OE1	1:A:920:GLN:HA	2.07	0.52
1:A:147:PRO:HG3	1:A:226:THR:HG23	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:GLY:C	1:A:631:THR:HG22	2.30	0.52
1:A:751:ARG:HD2	1:A:817:MET:HE1	1.90	0.52
1:A:106:VAL:HG13	1:A:107:TRP:H	1.75	0.52
1:A:272:TRP:CZ3	1:A:273:LEU:HD23	2.45	0.52
1:A:421:ASN:OD1	1:A:423:SER:N	2.43	0.52
1:A:457:THR:O	1:A:459:VAL:HG13	2.09	0.52
1:A:311:LEU:CD1	1:A:764:LEU:HD12	2.33	0.52
1:A:311:LEU:O	1:A:315:ILE:HG13	2.09	0.52
1:A:48:SER:OG	1:A:51:GLU:HG3	2.10	0.52
1:A:896:PRO:O	1:A:899:MET:HB2	2.09	0.52
1:A:114:ASN:HB3	1:A:117:GLU:HG2	1.92	0.52
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.40	0.52
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.90	0.52
1:A:389:TYR:CE2	1:A:436:LYS:HB2	2.44	0.52
1:A:758:LYS:HG3	1:A:828:LEU:HD21	1.93	0.52
1:A:737:ASP:C	1:A:739:ASN:H	2.13	0.51
1:A:482:GLU:OE1	1:A:573:ARG:NH1	2.43	0.51
1:A:920:GLN:HG3	1:A:924:ARG:NH1	2.25	0.51
1:A:865:VAL:O	1:A:865:VAL:HG22	2.09	0.51
1:A:18:VAL:HG23	1:A:24:LEU:HD23	1.91	0.51
1:A:244:GLN:CB	5:A:1101:HOH:O	2.58	0.51
1:A:23:GLY:HA2	1:A:150:ILE:HD13	1.92	0.51
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.40	0.51
1:A:973:ILE:O	1:A:976:PRO:HD2	2.10	0.51
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.92	0.51
1:A:389:TYR:CA	1:A:447:THR:HG21	2.41	0.51
1:A:612:GLN:O	1:A:615:ARG:HB2	2.11	0.51
1:A:77:TRP:O	1:A:78:PHE:HD1	1.94	0.51
1:A:102:ALA:O	1:A:106:VAL:HG12	2.11	0.50
1:A:529:ARG:NH2	1:A:568:ASP:OD1	2.44	0.50
1:A:338:SER:C	1:A:340:GLU:N	2.65	0.50
1:A:389:TYR:HA	1:A:447:THR:HG21	1.92	0.50
1:A:500:PRO:HG2	1:A:509:GLY:HA2	1.94	0.50
1:A:765:ILE:HG21	2:A:1001:1HT:H19	1.93	0.50
1:A:76:ALA:C	1:A:88:PHE:HE1	2.15	0.50
1:A:192:GLU:OE2	1:A:580:ASP:HA	2.12	0.50
1:A:512:MET:HB3	1:A:567:ARG:HB3	1.92	0.50
1:A:680:GLU:HG3	1:A:683:HIS:CE1	2.46	0.50
1:A:24:LEU:HG	1:A:149:ASP:CA	2.41	0.50
1:A:200:VAL:HG21	1:A:489:ARG:HH12	1.77	0.50
1:A:462:LEU:HD22	1:A:466:GLU:HG3	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ASP:O	1:A:582:SER:N	2.45	0.50
1:A:391:PRO:HD2	1:A:434:TYR:CD2	2.46	0.50
1:A:23:GLY:HA3	1:A:130:TYR:O	2.12	0.49
1:A:367:PHE:C	1:A:367:PHE:CD1	2.84	0.49
1:A:411:VAL:HG12	1:A:454:VAL:HG11	1.94	0.49
1:A:497:TYR:HD2	1:A:512:MET:HE3	1.77	0.49
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.94	0.49
1:A:770:GLY:HA3	1:A:844:VAL:HG22	1.93	0.49
1:A:615:ARG:HG2	1:A:615:ARG:NH1	2.28	0.49
1:A:855:TRP:CE3	1:A:896:PRO:HD3	2.47	0.49
1:A:70:CYS:O	1:A:71:ILE:C	2.51	0.49
1:A:720:MET:HB3	1:A:738:ASP:OD1	2.12	0.49
1:A:968:LEU:O	1:A:972:LYS:HG3	2.11	0.49
1:A:467:ARG:HG3	1:A:467:ARG:O	2.12	0.49
1:A:756:ASN:OD1	1:A:810:ASN:HB2	2.13	0.49
1:A:411:VAL:HB	1:A:454:VAL:HG11	1.94	0.49
1:A:28:GLN:HG2	1:A:31:ARG:NH2	2.28	0.49
1:A:267:ILE:CD1	2:A:1001:1HT:H2	2.38	0.48
1:A:148:GLY:O	1:A:222:ILE:HG13	2.13	0.48
1:A:478:LEU:HD22	1:A:479:MET:HG2	1.95	0.48
1:A:795:VAL:HA	1:A:799:THR:HB	1.94	0.48
1:A:163:ILE:HB	1:A:208:LEU:HB2	1.95	0.48
1:A:538:THR:HB	1:A:540:PRO:HD2	1.94	0.48
1:A:615:ARG:HG2	1:A:615:ARG:HH11	1.78	0.48
1:A:39:ASN:HB2	1:A:226:THR:HB	1.94	0.48
1:A:527:TYR:HD2	1:A:592:THR:CG2	2.25	0.48
1:A:628:ASN:CB	1:A:678:ARG:HH21	2.25	0.48
1:A:950:VAL:HG12	1:A:950:VAL:O	2.14	0.48
1:A:748:GLU:CA	1:A:817:MET:HE3	2.39	0.48
1:A:100:ALA:CB	3:A:1002:PTY:H311	2.43	0.48
1:A:345:THR:HG22	1:A:716:ILE:HD13	1.94	0.48
1:A:394:GLU:CD	1:A:396:LEU:HD21	2.34	0.48
1:A:192:GLU:CD	1:A:580:ASP:HA	2.34	0.48
1:A:863:PRO:CG	1:A:890:ILE:HG21	2.44	0.48
1:A:869:GLN:HB3	1:A:872:HIS:ND1	2.28	0.48
1:A:25:THR:OG1	1:A:28:GLN:HG3	2.13	0.48
1:A:500:PRO:CG	1:A:509:GLY:HA2	2.43	0.48
1:A:203:ASP:OD1	1:A:489:ARG:HD3	2.14	0.47
1:A:421:ASN:OD1	1:A:442:GLU:HB3	2.14	0.47
1:A:152:GLU:HG3	1:A:152:GLU:O	2.14	0.47
1:A:407:PHE:O	1:A:411:VAL:HG13	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLY:HA3	1:A:288:TRP:CD1	2.49	0.47
1:A:424:SER:O	1:A:437:VAL:HB	2.15	0.47
1:A:462:LEU:HD13	1:A:466:GLU:HG3	1.96	0.47
1:A:59:ASP:OD1	1:A:60:LEU:N	2.45	0.47
1:A:755:ASN:O	1:A:758:LYS:HB3	2.15	0.47
1:A:767:SER:O	1:A:771:GLU:HG3	2.14	0.47
1:A:77:TRP:HA	1:A:77:TRP:CE3	2.50	0.47
1:A:48:SER:N	1:A:51:GLU:OE1	2.44	0.47
1:A:966:GLN:O	1:A:969:MET:HB3	2.14	0.47
1:A:969:MET:HA	1:A:969:MET:CE	2.42	0.47
1:A:577:VAL:HG21	1:A:583:ARG:HH11	1.79	0.47
1:A:733:MET:HE1	1:A:746:ALA:HB1	1.96	0.47
1:A:969:MET:CE	1:A:972:LYS:HB2	2.45	0.47
1:A:294:TYR:O	1:A:297:LYS:HG2	2.15	0.47
1:A:417:CYS:SG	1:A:564:LEU:HD11	2.55	0.47
1:A:662:PRO:O	1:A:664:ALA:N	2.48	0.47
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.95	0.47
1:A:761:ILE:O	1:A:765:ILE:HG12	2.15	0.47
1:A:314:VAL:HG13	1:A:805:THR:HG22	1.96	0.47
1:A:993:GLU:H	1:A:993:GLU:CD	2.16	0.47
1:A:749:GLU:O	1:A:753:ILE:HG12	2.15	0.46
1:A:627:ASP:O	1:A:677:ALA:HB1	2.15	0.46
1:A:59:ASP:HB3	1:A:62:VAL:HG12	1.98	0.46
1:A:949:TYR:O	1:A:951:ASP:N	2.48	0.46
1:A:52:LEU:HD11	1:A:109:GLU:OE2	2.16	0.46
1:A:179:ILE:HG13	1:A:180:LEU:H	1.79	0.46
1:A:907:ILE:HG12	1:A:974:SER:HB2	1.97	0.46
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.73	0.46
1:A:941:MET:O	1:A:944:HIS:HB3	2.16	0.46
1:A:146:VAL:HG13	1:A:147:PRO:CD	2.45	0.46
1:A:380:ASN:O	1:A:382:PHE:CE1	2.69	0.46
1:A:558:THR:HB	1:A:635:ILE:CD1	2.46	0.46
1:A:402:ILE:HG22	1:A:403:ARG:N	2.29	0.46
1:A:483:PHE:CE1	1:A:578:LEU:HD22	2.48	0.46
1:A:926:PRO:HG2	1:A:929:VAL:HG23	1.97	0.46
1:A:658:PHE:CZ	1:A:666:GLN:HG2	2.51	0.46
1:A:636:CYS:SG	1:A:675:CYS:HB2	2.55	0.46
1:A:40:GLU:CD	1:A:143:ARG:HE	2.20	0.45
1:A:270:ALA:O	1:A:274:ILE:CG1	2.60	0.45
1:A:530:VAL:O	1:A:530:VAL:HG23	2.16	0.45
1:A:106:VAL:HG13	1:A:107:TRP:N	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HG	1:A:446:THR:HG21	1.98	0.45
1:A:44:GLU:HG3	1:A:117:GLU:OE2	2.16	0.45
1:A:24:LEU:CD1	1:A:149:ASP:HB3	2.46	0.45
1:A:392:GLU:O	1:A:451:LYS:HD3	2.17	0.45
1:A:394:GLU:CG	1:A:396:LEU:HD21	2.47	0.45
1:A:412:GLU:OE2	1:A:529:ARG:NE	2.46	0.45
1:A:59:ASP:HB3	1:A:62:VAL:CG1	2.47	0.45
1:A:870:LEU:HD12	1:A:891:PHE:CE1	2.48	0.45
1:A:193:PRO:HA	1:A:206:ASN:HD22	1.80	0.45
1:A:338:SER:O	1:A:340:GLU:N	2.50	0.45
1:A:39:ASN:CB	1:A:226:THR:HB	2.47	0.45
1:A:527:TYR:HB2	1:A:592:THR:HG22	0.56	0.45
1:A:836:ARG:HG2	1:A:984:LEU:HB3	1.99	0.45
1:A:358:THR:CG2	1:A:360:GLN:HG3	2.47	0.45
1:A:901:LEU:HD13	1:A:959:LEU:HD21	1.99	0.45
1:A:173:LEU:HD22	1:A:219:ALA:HB2	1.99	0.44
1:A:44:GLU:N	1:A:44:GLU:CD	2.70	0.44
1:A:122:TYR:HE2	1:A:726:VAL:HG23	1.81	0.44
1:A:748:GLU:CG	1:A:817:MET:HE3	2.42	0.44
1:A:791:GLN:HB3	1:A:901:LEU:HD11	1.97	0.44
1:A:668:GLU:HG3	1:A:672:ARG:CZ	2.47	0.44
1:A:680:GLU:CB	1:A:681:PRO:HD2	2.48	0.44
1:A:771:GLU:O	1:A:774:CYS:HB3	2.18	0.44
1:A:104:VAL:HG21	3:A:1002:PTY:HC11	1.99	0.44
1:A:166:LEU:HG	1:A:221:GLY:HA2	2.00	0.44
1:A:247:THR:CB	1:A:250:GLN:HG3	2.48	0.44
1:A:491:ARG:CB	1:A:585:MET:HG3	2.48	0.44
1:A:496:VAL:HG23	1:A:496:VAL:O	2.17	0.44
1:A:423:SER:OG	1:A:442:GLU:HB2	2.18	0.44
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.76	0.44
1:A:898:THR:HG21	1:A:960:LYS:O	2.17	0.44
1:A:949:TYR:O	1:A:950:VAL:C	2.56	0.44
1:A:971:LEU:CD2	1:A:975:LEU:HD11	2.47	0.44
1:A:836:ARG:HG2	1:A:984:LEU:HD13	1.99	0.44
1:A:103:ILE:O	1:A:106:VAL:HG13	2.18	0.44
1:A:152:GLU:HB3	1:A:220:LEU:HD12	1.99	0.44
1:A:159:VAL:HA	1:A:160:PRO:HD3	1.77	0.44
1:A:1:MET:CB	1:A:225:THR:HG22	2.37	0.44
1:A:606:GLU:O	1:A:741:SER:HB3	2.18	0.44
1:A:865:VAL:HG23	1:A:868:HIS:CE1	2.53	0.44
1:A:14:ALA:O	1:A:17:GLY:N	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLN:OE1	1:A:489:ARG:HD2	2.17	0.44
1:A:527:TYR:CG	1:A:592:THR:CG2	2.88	0.44
1:A:868:HIS:C	1:A:868:HIS:ND1	2.72	0.44
1:A:887:ASP:O	1:A:890:ILE:HG13	2.18	0.44
1:A:95:LEU:O	1:A:99:ILE:HG12	2.17	0.44
1:A:415:THR:HG22	1:A:475:ILE:HD13	2.00	0.43
1:A:877:THR:O	1:A:880:HIS:ND1	2.51	0.43
1:A:297:LYS:HA	1:A:300:VAL:HG22	2.00	0.43
1:A:586:GLU:OE1	1:A:586:GLU:N	2.50	0.43
1:A:122:TYR:HE2	1:A:726:VAL:HG21	1.83	0.43
1:A:394:GLU:OE1	1:A:401:PRO:HB3	2.18	0.43
1:A:50:TRP:CZ2	1:A:54:ILE:HD11	2.54	0.43
1:A:524:ARG:HD2	1:A:588:GLU:O	2.18	0.43
1:A:608:MET:SD	1:A:639:ILE:HA	2.58	0.43
1:A:668:GLU:O	1:A:671:ARG:HG2	2.18	0.43
1:A:679:VAL:HG13	1:A:683:HIS:CB	2.49	0.43
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.48	0.43
1:A:247:THR:CG2	1:A:340:GLU:OE1	2.65	0.43
1:A:555:GLY:O	1:A:557:ASP:N	2.51	0.43
1:A:886:LEU:C	1:A:886:LEU:HD12	2.38	0.43
1:A:258:GLU:O	1:A:261:SER:HB3	2.18	0.43
1:A:352:LYS:HE2	1:A:357:THR:HG21	2.01	0.43
1:A:737:ASP:C	1:A:739:ASN:N	2.72	0.43
1:A:737:ASP:O	1:A:739:ASN:N	2.51	0.43
1:A:285:GLY:O	1:A:288:TRP:HD1	2.01	0.43
1:A:550:LYS:O	1:A:554:THR:HB	2.18	0.43
1:A:617:ALA:HB1	1:A:751:ARG:NH1	2.33	0.43
1:A:691:LEU:O	1:A:696:GLU:HB2	2.19	0.43
1:A:528:VAL:O	1:A:528:VAL:HG23	2.18	0.43
1:A:355:THR:CG2	1:A:720:MET:SD	3.07	0.42
1:A:890:ILE:O	1:A:893:ALA:CB	2.67	0.42
1:A:19:SER:OG	1:A:22:THR:HB	2.19	0.42
1:A:349:CYS:HA	1:A:622:ILE:O	2.18	0.42
1:A:371:LYS:O	1:A:377:CYS:HA	2.18	0.42
1:A:420:CYS:SG	1:A:515:LYS:HE2	2.60	0.42
1:A:754:TYR:O	1:A:758:LYS:HB2	2.19	0.42
1:A:974:SER:C	1:A:976:PRO:HD2	2.39	0.42
1:A:150:ILE:HD12	1:A:150:ILE:N	2.34	0.42
1:A:500:PRO:O	1:A:501:ALA:CB	2.66	0.42
1:A:916:LEU:HD23	1:A:916:LEU:HA	1.80	0.42
1:A:969:MET:HE2	1:A:972:LYS:HB2	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:GLY:O	1:A:294:TYR:HB3	2.20	0.42
1:A:336:LEU:HB2	1:A:337:PRO:HD3	2.01	0.42
1:A:485:LEU:HD12	1:A:495:SER:OG	2.19	0.42
1:A:748:GLU:CB	1:A:817:MET:HE3	2.49	0.42
1:A:951:ASP:O	1:A:952:PRO:C	2.58	0.42
1:A:97:ILE:HD11	1:A:797:LEU:CD1	2.34	0.42
1:A:411:VAL:CG1	1:A:454:VAL:HG11	2.50	0.42
1:A:76:ALA:HB1	1:A:88:PHE:HD1	1.82	0.42
1:A:192:GLU:CD	1:A:580:ASP:CB	2.87	0.42
1:A:515:LYS:O	1:A:515:LYS:HG3	2.19	0.42
1:A:61:LEU:HD23	1:A:64:ILE:HD12	2.02	0.42
1:A:657:GLU:O	1:A:661:LEU:HG	2.20	0.42
1:A:404:SER:OG	1:A:452:MET:HB2	2.19	0.42
1:A:629:LYS:O	1:A:633:ILE:HG13	2.20	0.42
1:A:916:LEU:HB3	1:A:925:MET:HE1	2.00	0.42
1:A:128:LYS:HB2	1:A:128:LYS:HE3	1.88	0.41
1:A:365:LYS:HB3	1:A:552:TRP:CZ3	2.55	0.41
1:A:59:ASP:OD1	1:A:61:LEU:N	2.53	0.41
1:A:10:GLU:O	1:A:13:LEU:N	2.53	0.41
1:A:449:VAL:HG11	1:A:472:ASN:OD1	2.20	0.41
1:A:593:PHE:CZ	1:A:595:GLY:HA2	2.55	0.41
1:A:756:ASN:HB3	1:A:808:GLY:HA2	2.00	0.41
1:A:253:LEU:C	1:A:253:LEU:HD23	2.40	0.41
1:A:289:ILE:O	1:A:293:ILE:HG12	2.20	0.41
1:A:691:LEU:CB	1:A:698:THR:HG21	2.50	0.41
1:A:800:ASP:C	1:A:803:PRO:HD2	2.41	0.41
1:A:90:GLU:HB3	1:A:91:PRO:HD3	2.02	0.41
1:A:319:LEU:HB3	1:A:336:LEU:HB3	2.02	0.41
1:A:460:ARG:O	1:A:460:ARG:HD3	2.20	0.41
1:A:642:PHE:HD1	1:A:646:GLU:OE2	2.04	0.41
1:A:857:MET:HB2	1:A:866:THR:HA	2.02	0.41
1:A:901:LEU:O	1:A:901:LEU:HD23	2.20	0.41
1:A:178:SER:O	1:A:182:GLY:N	2.51	0.41
1:A:153:VAL:CB	1:A:214:ILE:HD11	2.50	0.41
1:A:452:MET:O	1:A:454:VAL:N	2.53	0.41
1:A:25:THR:HA	1:A:132:ALA:HB3	2.02	0.41
1:A:748:GLU:OE2	1:A:817:MET:HG3	2.20	0.41
1:A:834:PHE:CD1	1:A:834:PHE:C	2.94	0.41
1:A:992:LEU:HD12	1:A:993:GLU:HG2	2.03	0.41
1:A:146:VAL:CG1	1:A:147:PRO:HD2	2.50	0.41
1:A:90:GLU:N	1:A:91:PRO:HD2	2.36	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:SER:C	1:A:340:GLU:H	2.23	0.41
1:A:455:PHE:O	1:A:456:ASN:HB2	2.20	0.41
1:A:433:VAL:CG1	1:A:434:TYR:N	2.83	0.41
1:A:669:ALA:O	1:A:672:ARG:HG2	2.21	0.41
1:A:692:GLN:C	1:A:694:TYR:H	2.24	0.41
1:A:916:LEU:CD1	1:A:927:PRO:HA	2.51	0.41
1:A:75:LEU:HD11	1:A:297:LYS:N	2.36	0.41
1:A:105:GLY:CA	3:A:1002:PTY:HC21	2.51	0.41
1:A:924:ARG:O	1:A:926:PRO:HD3	2.21	0.41
1:A:367:PHE:CE1	1:A:379:LEU:CD2	3.05	0.40
1:A:363:VAL:HG13	1:A:597:VAL:HG13	2.03	0.40
1:A:637:ARG:NH1	1:A:643:GLY:O	2.54	0.40
1:A:916:LEU:HD21	1:A:933:LEU:HD22	2.03	0.40
1:A:174:ARG:HA	1:A:187:VAL:O	2.21	0.40
1:A:247:THR:HG22	1:A:250:GLN:HG3	2.02	0.40
1:A:580:ASP:C	1:A:582:SER:N	2.73	0.40
1:A:683:HIS:O	1:A:684:LYS:C	2.57	0.40
1:A:77:TRP:HE3	1:A:77:TRP:HA	1.85	0.40
1:A:802:LEU:HB3	1:A:936:SER:HB2	2.02	0.40
1:A:811:PRO:HA	1:A:812:PRO:HD3	1.71	0.40
1:A:192:GLU:OE2	1:A:580:ASP:CA	2.70	0.40
1:A:635:ILE:O	1:A:639:ILE:HG12	2.21	0.40
1:A:271:VAL:HA	1:A:274:ILE:HG12	2.04	0.40
1:A:654:THR:HG23	1:A:656:ARG:N	2.35	0.40
1:A:703:ASP:OD1	1:A:704:GLY:N	2.55	0.40
1:A:907:ILE:HD11	1:A:974:SER:HA	2.03	0.40
1:A:957:PHE:O	1:A:958:LYS:HB2	2.21	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%)	865 (87%)	106 (11%)	21 (2%)	7	37

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	THR
1	A	950	VAL
1	A	453	ASN
1	A	501	ALA
1	A	581	SER
1	A	606	GLU
1	A	663	LEU
1	A	869	GLN
1	A	285	GLY
1	A	457	THR
1	A	556	ARG
1	A	178	SER
1	A	520	GLY
1	A	738	ASP
1	A	951	ASP
1	A	81	GLY
1	A	160	PRO
1	A	470	ALA
1	A	605	LYS
1	A	864	GLY
1	A	975	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	840/840 (100%)	817 (97%)	23 (3%)	44	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	49	LEU
1	A	101	ASN
1	A	135	LYS
1	A	207	MET
1	A	247	THR
1	A	298	ILE
1	A	360	GLN
1	A	364	CYS
1	A	367	PHE
1	A	375	ASP
1	A	396	LEU
1	A	411	VAL
1	A	490	ASP
1	A	596	VAL
1	A	606	GLU
1	A	666	GLN
1	A	844	VAL
1	A	868	HIS
1	A	869	GLN
1	A	925	MET
1	A	969	MET
1	A	993	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	990	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is 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	PTY	A	1002	-	23,23,49	1.77	2 (8%)	26,28,54	1.75	4 (15%)
2	1HT	A	1001	-	50,53,53	4.51	23 (46%)	52,78,78	3.58	27 (51%)

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	PTY	A	1002	-	-	9/27/27/53	-
2	1HT	A	1001	-	-	18/41/107/107	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	1HT	CBN-CBQ	23.43	1.54	1.34
3	A	1002	PTY	O30-C30	7.09	1.43	1.22
2	A	1001	1HT	OAO-CBP	6.99	1.36	1.20
2	A	1001	1HT	OBG-CBX	-6.75	1.36	1.48
2	A	1001	1HT	CBW-CBY	-6.75	1.46	1.55
2	A	1001	1HT	OBD-CBT	-6.60	1.34	1.44
2	A	1001	1HT	OBC-CBR	-5.97	1.36	1.46
2	A	1001	1HT	OBE-CBS	-5.66	1.34	1.44
2	A	1001	1HT	OBF-CBU	-5.55	1.37	1.46
2	A	1001	1HT	OBF-CBP	4.93	1.42	1.35
2	A	1001	1HT	CAQ-CBJ	4.63	1.60	1.31
2	A	1001	1HT	CAG-CBN	-4.31	1.43	1.50
2	A	1001	1HT	CBY-CBU	-3.95	1.47	1.53
2	A	1001	1HT	OBE-CBO	3.74	1.43	1.34
2	A	1001	1HT	CAF-CBJ	3.70	1.59	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	1HT	CBS-CBN	3.68	1.55	1.50
3	A	1002	PTY	O4-C30	3.59	1.43	1.33
2	A	1001	1HT	CBO-CBJ	3.55	1.62	1.50
2	A	1001	1HT	CBY-CBR	2.65	1.58	1.52
2	A	1001	1HT	OBC-CBK	2.60	1.41	1.34
2	A	1001	1HT	OBH-CBM	2.53	1.41	1.33
2	A	1001	1HT	OAP-CBW	-2.49	1.38	1.42
2	A	1001	1HT	OBH-CBY	-2.49	1.40	1.44
2	A	1001	1HT	CBV-CBT	-2.14	1.51	1.54
2	A	1001	1HT	CBB-CBX	-2.03	1.50	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	1HT	OBF-CBP-OAO	-12.97	104.43	121.62
2	A	1001	1HT	CAG-CBN-CBQ	-10.39	103.88	129.82
2	A	1001	1HT	OAO-CBP-CBW	-9.16	119.08	128.28
3	A	1002	PTY	O4-C30-O30	-6.00	108.45	123.59
2	A	1001	1HT	CBB-CBR-CBY	5.66	122.70	115.38
2	A	1001	1HT	CBY-CBU-CBQ	5.50	129.00	115.28
2	A	1001	1HT	CBY-OBH-CBM	4.79	131.51	119.97
2	A	1001	1HT	CAI-CBX-CBB	4.01	118.42	110.29
3	A	1002	PTY	O30-C30-C31	-4.01	108.09	123.73
2	A	1001	1HT	CBX-CBV-CBQ	-3.86	110.64	115.26
2	A	1001	1HT	OBE-CBO-CBJ	3.84	121.16	111.52
2	A	1001	1HT	OBH-CBM-OAM	-3.72	115.81	124.97
2	A	1001	1HT	CBS-CBN-CBQ	-3.37	96.98	107.85
3	A	1002	PTY	O7-C8-C11	3.21	119.75	110.80
2	A	1001	1HT	CAG-CBN-CBS	-3.19	116.10	121.27
2	A	1001	1HT	CBX-OBG-CBI	3.18	129.08	121.53
2	A	1001	1HT	CAF-CBJ-CAQ	-3.07	110.55	123.20
2	A	1001	1HT	OBH-CBM-CAZ	3.05	116.08	110.71
2	A	1001	1HT	OBC-CBK-OAK	-2.87	116.75	123.70
2	A	1001	1HT	OAM-CBM-CAZ	-2.77	112.93	123.73
2	A	1001	1HT	OBG-CBI-OAJ	-2.76	118.53	123.61
2	A	1001	1HT	OBE-CBO-OAN	-2.62	118.32	123.32
2	A	1001	1HT	OBG-CBI-CAE	2.60	115.41	110.68
2	A	1001	1HT	OAP-CBW-CAH	-2.56	104.88	109.59
3	A	1002	PTY	C6-O7-C8	-2.51	111.60	117.79
2	A	1001	1HT	OBC-CBR-CBB	2.46	111.03	106.63
2	A	1001	1HT	OAN-CBO-CBJ	-2.41	117.66	125.21
2	A	1001	1HT	OBC-CBR-CBY	-2.38	102.04	106.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	1HT	OBD-CBL-CBA	2.33	116.51	111.50
2	A	1001	1HT	OAJ-CBI-CAE	-2.02	117.44	124.81
2	A	1001	1HT	OAK-CBK-CAY	-2.01	115.89	123.73

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	PTY	C3-O11-P1-O12
2	A	1001	1HT	CBR-CBY-OBH-CBM
2	A	1001	1HT	CBU-CBY-OBH-CBM
2	A	1001	1HT	OAM-CBM-OBH-CBY
2	A	1001	1HT	CAZ-CBM-OBH-CBY
2	A	1001	1HT	CAF-CBJ-CBO-OAN
2	A	1001	1HT	CAA-CAQ-CBJ-CBO
2	A	1001	1HT	CAA-CAQ-CBJ-CAF
3	A	1002	PTY	O30-C30-O4-C1
2	A	1001	1HT	OAN-CBO-OBE-CBS
3	A	1002	PTY	C31-C30-O4-C1
3	A	1002	PTY	O4-C1-C6-O7
2	A	1001	1HT	OAJ-CBI-OBG-CBX
3	A	1002	PTY	C3-O11-P1-O14
2	A	1001	1HT	OAK-CBK-OBC-CBR
2	A	1001	1HT	CAU-CAV-CAW-CAX
2	A	1001	1HT	CBJ-CBO-OBE-CBS
2	A	1001	1HT	CBA-CBL-OB-DBT
2	A	1001	1HT	CAB-CAR-CAU-CAV
2	A	1001	1HT	CAW-CAX-CBA-CBL
3	A	1002	PTY	O4-C1-C6-C5
3	A	1002	PTY	C3-O11-P1-O13
3	A	1002	PTY	C5-O14-P1-O11
2	A	1001	1HT	CAF-CBJ-CBO-OBE
2	A	1001	1HT	CAS-CAY-CBK-OBC
3	A	1002	PTY	O4-C30-C31-C32
2	A	1001	1HT	CAT-CAZ-CBM-OAM

There are no ring outliers.

2 monomers are involved in 12 short contacts:

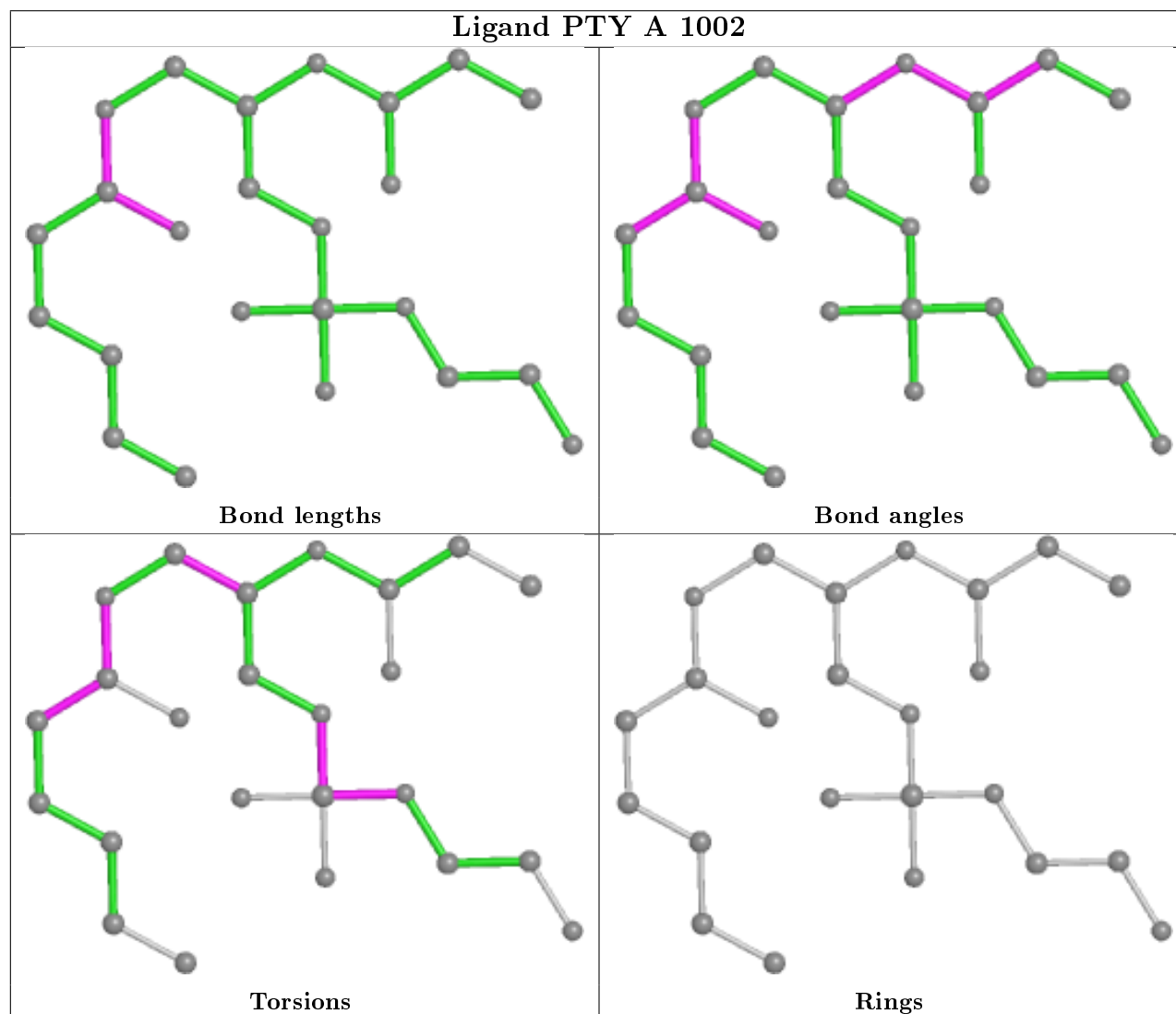
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	PTY	4	0

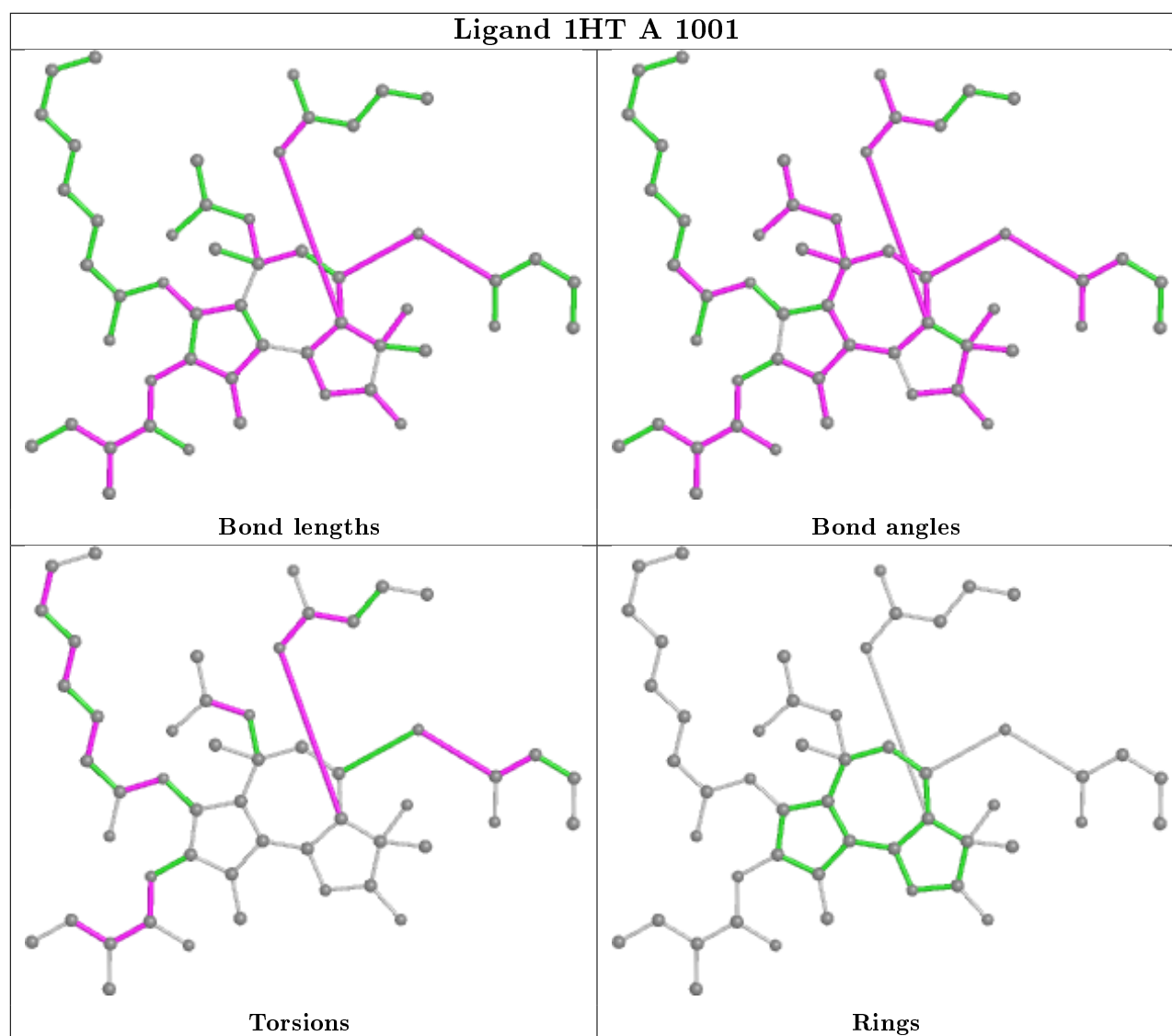
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	1HT	8	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	994/994 (100%)	-0.04	37 (3%) 41 26	30, 91, 164, 257	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	SER	5.9
1	A	504	SER	5.4
1	A	46	GLY	5.2
1	A	81	GLY	5.1
1	A	506	ALA	4.7
1	A	47	LYS	3.8
1	A	50	TRP	3.8
1	A	507	ALA	3.8
1	A	878	GLU	3.7
1	A	951	ASP	3.5
1	A	48	SER	3.5
1	A	888	CYS	3.2
1	A	428	ASN	3.1
1	A	435	GLU	3.1
1	A	508	VAL	3.0
1	A	430	THR	3.0
1	A	994	GLY	2.9
1	A	505	ARG	2.9
1	A	796	ASN	2.8
1	A	767	SER	2.8
1	A	420	CYS	2.7
1	A	768	ASN	2.7
1	A	284	HIS	2.7
1	A	109	GLU	2.7
1	A	280	ASN	2.6
1	A	80	GLU	2.5
1	A	876	CYS	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	183	GLU	2.3
1	A	285	GLY	2.2
1	A	881	PRO	2.2
1	A	877	THR	2.2
1	A	31	ARG	2.2
1	A	509	GLY	2.1
1	A	106	VAL	2.1
1	A	766	SER	2.1
1	A	429	GLU	2.0
1	A	434	TYR	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

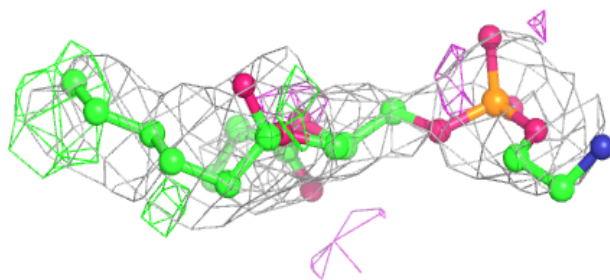
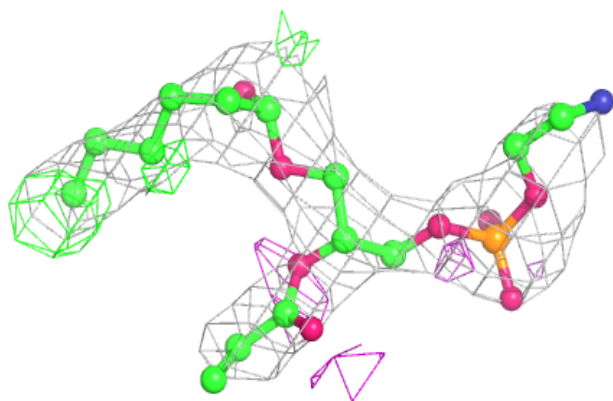
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PTY	A	1002	24/50	0.72	0.44	114,124,132,133	0
2	1HT	A	1001	51/51	0.85	0.41	152,152,152,152	0
4	K	A	1003	1/1	0.94	0.15	78,78,78,78	0

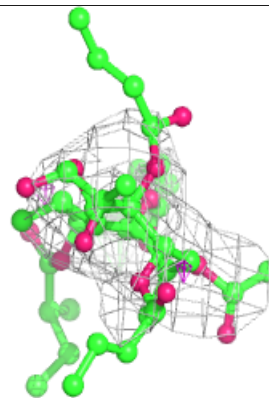
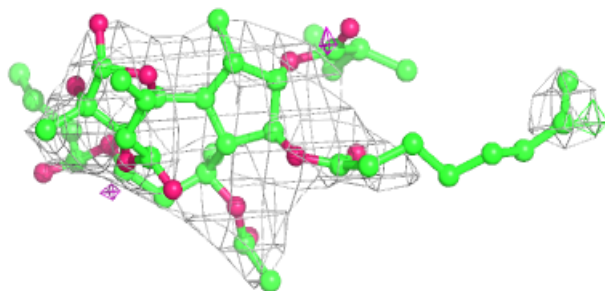
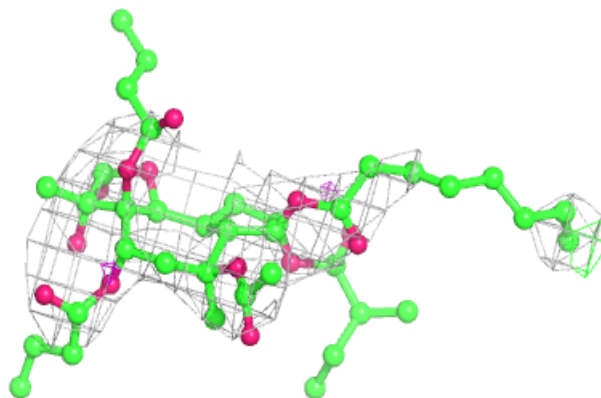
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PTY A 1002:**

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

**Electron density around 1HT A 1001:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.