



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:07 PM UTC

PDB ID : 4J2T / pdb_00004j2t
Title : Inhibitor-bound Ca²⁺ ATPase
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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

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

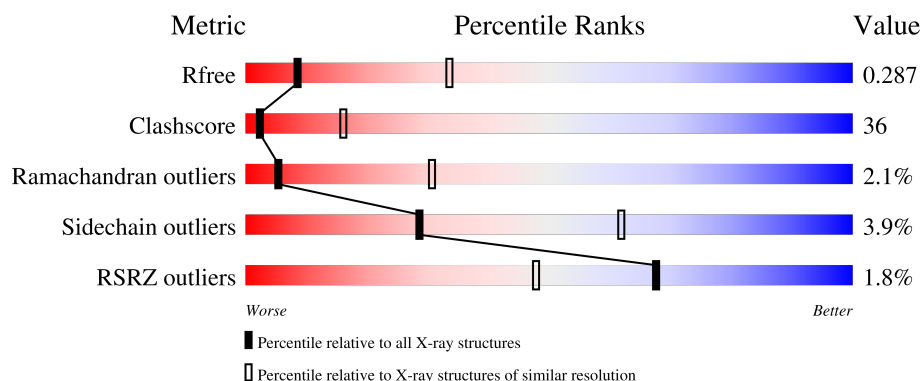
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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](#)

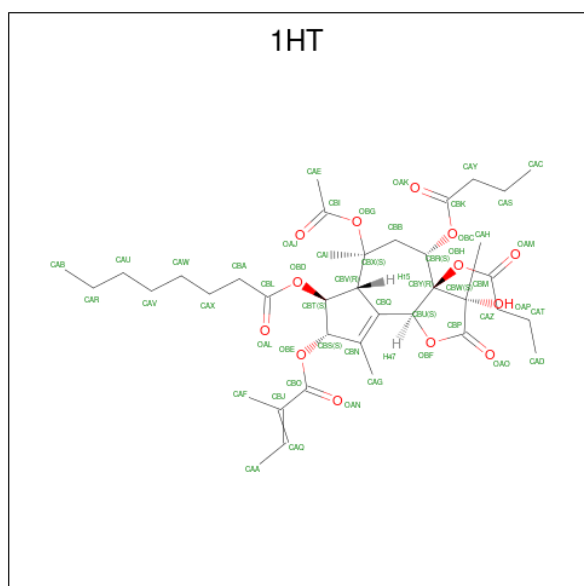
There are 5 unique types of molecules in this entry. The entry contains 7748 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

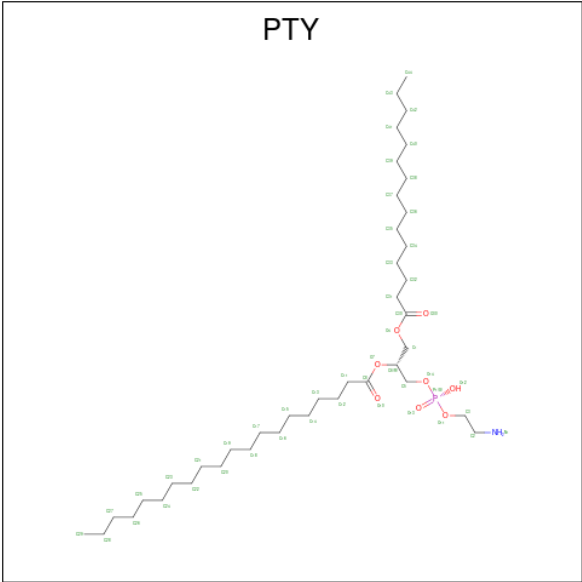
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	994	7671	4876	1287	1451	57	0	0	0

- 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 (CCD ID: 1HT) (formula: C₃₈H₅₆O₁₃).



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

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



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 (CCD ID: 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		



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	70.90Å 70.90Å 587.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.71 – 3.20 28.71 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.71-3.20) 99.4 (28.71-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.260 , 0.286 0.263 , 0.287	Depositor DCC
R_{free} test set	2000 reflections (6.34%)	wwPDB-VP
Wilson B-factor (Å ²)	73.5	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	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 ²)	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.*

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: PTY, K, 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	0.59	5/7812 (0.1%)	1.06	44/10592 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	ASN	C-N	-8.76	1.22	1.33
1	A	345	THR	C-N	-7.93	1.22	1.33
1	A	744	VAL	C-N	7.16	1.43	1.33
1	A	741	SER	C-N	-6.72	1.24	1.34
1	A	601	ASP	C-N	6.36	1.40	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	870	LEU	N-CA-C	-13.06	95.78	112.23
1	A	798	VAL	N-CA-C	8.79	119.74	111.48
1	A	351	ASP	N-CA-C	-7.44	100.71	110.53
1	A	628	ASN	N-CA-C	-7.04	101.05	110.55
1	A	498	CYS	N-CA-C	6.87	120.70	109.24
1	A	838	MET	N-CA-C	-6.69	103.99	111.28
1	A	474	VAL	N-CA-C	-6.50	104.00	110.30
1	A	532	THR	N-CA-C	-6.49	105.94	114.31
1	A	389	TYR	N-CA-C	-6.36	106.23	112.97
1	A	163	ILE	N-CA-C	6.34	117.72	108.53
1	A	179	ILE	N-CA-C	6.12	116.78	110.36
1	A	561	CYS	N-CA-C	5.82	118.97	109.59
1	A	71	ILE	N-CA-C	-5.81	104.00	110.62
1	A	953	LEU	N-CA-C	5.73	120.28	112.55
1	A	121	GLU	N-CA-C	-5.68	106.31	113.18
1	A	862	GLY	CA-C-N	5.66	126.91	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	862	GLY	C-N-CA	5.66	126.91	119.84
1	A	683	HIS	N-CA-C	5.63	117.89	111.02
1	A	207	MET	N-CA-C	5.57	118.47	109.40
1	A	893	ALA	CA-C-N	5.57	126.80	119.84
1	A	893	ALA	C-N-CA	5.57	126.80	119.84
1	A	798	VAL	CB-CA-C	-5.56	106.98	111.71
1	A	468	ALA	N-CA-C	5.55	117.01	111.07
1	A	992	LEU	N-CA-C	-5.53	102.21	110.23
1	A	122	TYR	O-C-N	5.51	129.12	122.35
1	A	951	ASP	N-CA-C	5.45	121.84	109.81
1	A	514	VAL	N-CA-C	5.41	117.11	108.89
1	A	338	SER	N-CA-C	5.40	118.09	111.82
1	A	521	VAL	N-CA-C	5.40	116.77	110.62
1	A	504	SER	N-CA-C	-5.39	105.31	113.51
1	A	122	TYR	CA-C-N	-5.38	114.24	122.42
1	A	122	TYR	C-N-CA	-5.38	114.24	122.42
1	A	679	VAL	N-CA-C	5.38	115.59	107.80
1	A	600	LEU	N-CA-C	5.37	118.15	109.40
1	A	601	ASP	O-C-N	5.30	126.46	120.68
1	A	400	LYS	CA-C-N	5.19	125.19	119.90
1	A	400	LYS	C-N-CA	5.19	125.19	119.90
1	A	841	GLY	N-CA-C	-5.17	106.50	112.50
1	A	990	ASN	N-CA-C	5.14	119.59	112.45
1	A	3	ALA	N-CA-C	-5.11	104.00	111.30
1	A	744	VAL	O-C-N	5.09	126.88	121.89
1	A	909	MET	N-CA-C	-5.08	105.83	112.23
1	A	593	PHE	CA-C-N	-5.05	117.76	122.66
1	A	593	PHE	C-N-CA	-5.05	117.76	122.66

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	555	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	555	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 36.

All (555) 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:909:MET:HE3	1:A:937:ILE:HG12	1.49	0.95
1:A:311:LEU:HD13	1:A:764:LEU:HD12	1.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:C	1:A:108:GLN:H	1.88	0.80
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:326:MET:HE1	1:A:339:VAL:HG13	1.61	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
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: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:748:GLU:HA	1:A:817:MET:HE3	1.66	0.76
1:A:969:MET:HA	1:A:969:MET:HE3	1.68	0.75
1:A:106:VAL:C	1:A:108:GLN:N	2.41	0.74
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: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:361:MET:HE3	1:A:599:MET:HG3	1.72	0.72
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: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:441:THR:HA	1:A:599:MET:HE1	1.73	0.70
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:748:GLU:HG3	1:A:817:MET:HE3	1.73	0.70
1:A:535:VAL:CG1	1:A:536:PRO:HD2	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:LEU:O	1:A:873:PHE:HB3	1.92	0.69
1:A:44:GLU:CD	1:A:44:GLU:H	1.99	0.69
1:A:751:ARG:HD2	1:A:817:MET:HE2	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:606:GLU:H	1:A:606:GLU:CD	2.00	0.68
1:A:813:ASP:O	1:A:816:ILE:HG13	1.93	0.68
1:A:97:ILE:CD1	1:A:797:LEU:HD11	2.21	0.68
1:A:969:MET:O	1:A:973:ILE:HG13	1.93	0.68
1:A:971:LEU:HD22	1:A:975:LEU:HD11	1.74	0.68
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.29	0.68
1:A:455:PHE:HB2	1:A:457:THR:HG23	1.74	0.68
1:A:79:GLU:HG3	1:A:87:ALA:CB	2.25	0.67
1:A:530:VAL:HG23	1:A:533:THR:OG1	1.95	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:1001:1HT: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:733:MET:HE1	1:A:746:ALA:HB1	1.78	0.65
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:527:TYR:CB	1:A:592:THR:CG2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:MET:HE3	1:A:599:MET:HE2	1.80	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:304:VAL:HB	1:A:793:LEU:CD2	2.24	0.64
1:A:484:THR:HG22	1:A:496:VAL:HG12	1.80	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:361:MET:HE2	1:A:441:THR:HG22	1.78	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:80:GLU:HB2	1:A:83:GLU:OE1	1.97	0.63
1:A:192:GLU:OE1	1:A:580:ASP:CB	2.47	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:925:MET:HE3	1:A:929:VAL:HG11	1.81	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:65:LEU:CG	1:A:307:ILE:HD12	2.30	0.62
1:A:263:VAL:HG11	2:A:1001:1HT:OAN	2.00	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:45:GLU:OE2	1:A:47:LYS:HG3	2.00	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: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:177:GLN:O	1:A:178:SER:C	2.44	0.60
1:A:383:SER:C	1:A:384:ILE:HD12	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:519:GLU:CD	1:A:519:GLU:H	2.11	0.58
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
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:355:THR:HG21	1:A:720:MET:CE	2.33	0.58
1:A:507:ALA:O	1:A:508:VAL:HG22	2.04	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:86:THR:CG2	1:A:955:MET:HE3	2.34	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:369:ILE:HD13	1:A:528:VAL:HB	1.86	0.57
1:A:397:LYS:CB	1:A:402:ILE:HD11	2.34	0.57
1:A:553:GLY:C	1:A:631:THR:HG22	2.30	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:79:GLU:HG3	1:A:87:ALA:HB1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:THR:HG23	1:A:656:ARG:H	1.69	0.56
1:A:79:GLU:HG3	1:A:87:ALA:HB2	1.88	0.56
1:A:623:MET:HE1	1:A:635:ILE:HG22	1.87	0.56
1:A:737:ASP:C	1:A:739:ASN:H	2.13	0.56
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.87	0.56
1:A:61:LEU:CD2	1:A:260:LEU:HD23	2.36	0.56
1:A:163:ILE:C	1:A:207:MET:HE3	2.31	0.56
1:A:483:PHE:CD1	1:A:578:LEU:HD22	2.40	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: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
1:A:247:THR:CG2	1:A:250:GLN:HG3	2.36	0.55
1:A:751:ARG:HD2	1:A:817:MET:HE1	1.87	0.55
1:A:979:GLY:O	1:A:983:ILE:HG13	2.06	0.55
1:A:648:VAL:HG12	1:A:648:VAL:O	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:76:ALA:C	1:A:88:PHE:HE1	2.15	0.54
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:122:TYR:HE2	1:A:726:VAL:CG2	2.19	0.54
1:A:367:PHE:CD1	1:A:367:PHE:C	2.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:CYS:O	1:A:71:ILE:C	2.51	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:338:SER:C	1:A:340:GLU:N	2.65	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:163:ILE:O	1:A:207:MET:HE3	2.08	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: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:394:GLU:CD	1:A:396:LEU:HD21	2.34	0.53
1:A:777:LEU:HB2	1:A:849:VAL:HG21	1.89	0.53
1:A:192:GLU:CD	1:A:580:ASP:HA	2.34	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
1:A:433:VAL:HG12	1:A:434:TYR:N	2.24	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:311:LEU:CD1	1:A:764:LEU:HD12	2.33	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:288:TRP:H	1:A:288:TRP:CD1	2.27	0.52
1:A:311:LEU:O	1:A:315:ILE:HG13	2.09	0.52
1:A:993:GLU:H	1:A:993:GLU:CD	2.16	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:90:GLU:HB3	1:A:91:PRO:CD	2.40	0.52
1:A:114:ASN:HB3	1:A:117:GLU:HG2	1.92	0.52
1:A:528:VAL:HG12	1:A:537:MET:HE2	1.91	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:VAL:HG22	1:A:865:VAL:O	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:497:TYR:CD2	1:A:512:MET:HE3	2.46	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:748:GLU:CA	1:A:817:MET:HE3	2.37	0.50
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:40:GLU:CD	1:A:143:ARG:HE	2.20	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: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
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:411:VAL:HG12	1:A:454:VAL:HG11	1.94	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:NH1	1:A:615:ARG:HG2	2.28	0.49
1:A:855:TRP:CE3	1:A:896:PRO:HD3	2.47	0.49
1:A:44:GLU:CD	1:A:44:GLU:N	2.70	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:O	1:A:467:ARG:HG3	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:748:GLU:CG	1:A:817:MET:HE3	2.42	0.49
1:A:28:GLN:HG2	1:A:31:ARG:NH2	2.28	0.49
1:A:148:GLY:O	1:A:222:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:CD1	2:A:1001:1HT:H2	2.38	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:949:TYR:O	1:A:950:VAL:C	2.56	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:868:HIS:ND1	1:A:868:HIS:C	2.72	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:O	1:A:950:VAL:HG12	2.14	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:326:MET:HE2	1:A:749:GLU:HB3	1.96	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:886:LEU:C	1:A:886:LEU:HD12	2.38	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:O	1:A:152:GLU:HG3	2.14	0.47
1:A:407:PHE:O	1:A:411:VAL:HG13	2.13	0.47
1:A:59:ASP:OD1	1:A:60:LEU:N	2.45	0.47
1:A:77:TRP:HA	1:A:77:TRP:CE3	2.50	0.47
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: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: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:192:GLU:CD	1:A:580:ASP:CB	2.87	0.47
1:A:497:TYR:HD2	1:A:512:MET:HE3	1.79	0.47
1:A:623:MET:HE1	1:A:635:ILE:CG2	2.44	0.47
1:A:969:MET:HA	1:A:969:MET:CE	2.42	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:577:VAL:HG21	1:A:583:ARG:HH11	1.79	0.47
1:A:969:MET:CE	1:A:972:LYS:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:951:ASP:O	1:A:952:PRO:C	2.58	0.47
1:A:314:VAL:HG13	1:A:805:THR:HG22	1.96	0.47
1:A:974:SER:C	1:A:976:PRO:HD2	2.39	0.47
1:A:749:GLU:O	1:A:753:ILE:HG12	2.15	0.46
1:A:239:MET:HE3	1:A:712:LYS:HD2	1.96	0.46
1:A:333:VAL:HG22	1:A:733:MET:HE3	1.98	0.46
1:A:627:ASP:O	1:A:677:ALA:HB1	2.15	0.46
1:A:737:ASP:C	1:A:739:ASN:N	2.72	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:253:LEU:HD23	1:A:253:LEU:C	2.40	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:692:GLN:C	1:A:694:TYR:H	2.24	0.46
1:A:834:PHE:C	1:A:834:PHE:CD1	2.94	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:270:ALA:O	1:A:274:ILE:CG1	2.60	0.45
1:A:338:SER:C	1:A:340:GLU:H	2.23	0.45
1:A:530:VAL:HG23	1:A:530:VAL:O	2.16	0.45
1:A:800:ASP:C	1:A:803:PRO:HD2	2.41	0.45
1:A:106:VAL:HG13	1:A:107:TRP:N	2.31	0.45
1:A:44:GLU:HG3	1:A:117:GLU:OE2	2.16	0.45
1:A:425:LEU:HG	1:A:446:THR:HG21	1.98	0.45
1:A:24:LEU:CD1	1:A:149:ASP:HB3	2.46	0.45
1:A:319:LEU:CD2	1:A:757:MET:HE1	2.47	0.45
1:A:580:ASP:C	1:A:582:SER:N	2.73	0.45
1:A:683:HIS:O	1:A:684:LYS:C	2.57	0.45
1:A:392:GLU:O	1:A:451:LYS:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:THR:CA	1:A:599:MET:HE1	2.45	0.45
1:A:59:ASP:HB3	1:A:62:VAL:CG1	2.47	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:870:LEU:HD12	1:A:891:PHE:CE1	2.48	0.45
1:A:39:ASN:CB	1:A:226:THR:HB	2.47	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: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:456:ASN:O	1:A:457:THR:C	2.60	0.44
1:A:563:ALA:C	1:A:564:LEU:HD23	2.42	0.44
1:A:122:TYR:HE2	1:A:726:VAL:HG23	1.81	0.44
1:A:412:GLU:O	1:A:413:LEU:C	2.60	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:864:GLY:C	1:A:866:THR:H	2.23	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:873:PHE:CD1	1:A:873:PHE:C	2.94	0.44
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.76	0.44
1:A:423:SER:OG	1:A:442:GLU:HB2	2.18	0.44
1:A:836:ARG:HG2	1:A:984:LEU:HD13	1.99	0.44
1:A:898:THR:HG21	1:A:960:LYS:O	2.17	0.44
1:A:971:LEU:CD2	1:A:975:LEU:HD11	2.47	0.44
1:A:1:MET:CB	1:A:225:THR:HG22	2.37	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: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:876:CYS:C	1:A:888:CYS:SG	3.01	0.44
1:A:14:ALA:O	1:A:17:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:O	1:A:99:ILE:HG12	2.17	0.44
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:887:ASP:O	1:A:890:ILE:HG13	2.18	0.44
1:A:415:THR:HG22	1:A:475:ILE:HD13	2.00	0.43
1:A:452:MET:O	1:A:453:ASN:C	2.60	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:N	1:A:586:GLU:OE1	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:555:GLY:C	1:A:557:ASP:N	2.77	0.43
1:A:748:GLU:CB	1:A:817:MET:HE3	2.48	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: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: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:141:LYS:O	1:A:142:ALA:C	2.62	0.43
1:A:338:SER:O	1:A:339:VAL:C	2.62	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:58:GLU:O	1:A:59:ASP:C	2.61	0.42
1:A:349:CYS:HA	1:A:622:ILE:O	2.18	0.42
1:A:359:ASN:O	1:A:359:ASN:CG	2.62	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:150:ILE:HD12	1:A:150:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:PRO:O	1:A:501:ALA:CB	2.66	0.42
1:A:534:ARG:C	1:A:535:VAL:HG23	2.45	0.42
1:A:916:LEU:HD23	1:A:916:LEU:HA	1.80	0.42
1:A:97:ILE:HD11	1:A:797:LEU:CD1	2.34	0.42
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:76:ALA:HB1	1:A:88:PHE:HD1	1.82	0.42
1:A:388:THR:C	1:A:390:ALA:H	2.26	0.42
1:A:411:VAL:CG1	1:A:454:VAL:HG11	2.50	0.42
1:A:61:LEU:HD23	1:A:64:ILE:HD12	2.02	0.42
1:A:331:ALA:HB1	1:A:733:MET:HE2	2.01	0.42
1:A:515:LYS:O	1:A:515:LYS:HG3	2.19	0.42
1:A:657:GLU:O	1:A:661:LEU:HG	2.20	0.42
1:A:39:ASN:CG	1:A:226:THR:HB	2.45	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:692:GLN:C	1:A:694:TYR:N	2.78	0.42
1:A:931:ILE:O	1:A:932:TRP:C	2.61	0.42
1:A:969:MET:HE2	1:A:972:LYS:HB2	2.01	0.42
1:A:59:ASP:OD1	1:A:61:LEU:N	2.53	0.41
1:A:128:LYS:HE3	1:A:128:LYS:HB2	1.88	0.41
1:A:365:LYS:HB3	1:A:552:TRP:CZ3	2.55	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:90:GLU:HB3	1:A:91:PRO:HD3	2.02	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:760:PHE:CD1	1:A:760:PHE:C	2.99	0.41
1:A:10:GLU:CD	1:A:10:GLU:H	2.28	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:153:VAL:CB	1:A:214:ILE:HD11	2.50	0.41
1:A:178:SER:O	1:A:182:GLY:N	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:GLU:OE2	1:A:817:MET:HG3	2.20	0.41
1:A:992:LEU:HD12	1:A:993:GLU:HG2	2.03	0.41
1:A:90:GLU:N	1:A:91:PRO:HD2	2.36	0.41
1:A:146:VAL:CG1	1:A:147:PRO:HD2	2.50	0.41
1:A:427:PHE:CD1	1:A:427:PHE:C	2.99	0.41
1:A:455:PHE:O	1:A:456:ASN:HB2	2.20	0.41
1:A:579:ASP:C	1:A:579:ASP:OD1	2.62	0.41
1:A:75:LEU:HD11	1:A:297:LYS:N	2.36	0.41
1:A:259:GLN:O	1:A:260:LEU:C	2.61	0.41
1:A:263:VAL:O	1:A:264:ILE:C	2.63	0.41
1:A:415:THR:O	1:A:416:ILE:C	2.64	0.41
1:A:433:VAL:CG1	1:A:434:TYR:N	2.83	0.41
1:A:580:ASP:O	1:A:581:SER:C	2.63	0.41
1:A:669:ALA:O	1:A:672:ARG:HG2	2.21	0.41
1:A:916:LEU:CD1	1:A:927:PRO:HA	2.51	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:363:VAL:HG13	1:A:597:VAL:HG13	2.03	0.40
1:A:367:PHE:CE1	1:A:379:LEU:CD2	3.05	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:77:TRP:HA	1:A:77:TRP:HE3	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:389:TYR:C	1:A:447:THR:HG21	2.47	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

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%)	865 (87%)	106 (11%)	21 (2%)	5	31

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%)	807 (96%)	33 (4%)	28	62

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	42	PRO
1	A	49	LEU
1	A	74	VAL
1	A	106	VAL
1	A	135	LYS
1	A	175	VAL
1	A	191	THR
1	A	232	ILE
1	A	234	LYS
1	A	246	LYS
1	A	247	THR
1	A	298	ILE
1	A	304	VAL
1	A	323	THR
1	A	358	THR
1	A	360	GLN
1	A	364	CYS
1	A	367	PHE
1	A	396	LEU
1	A	411	VAL
1	A	466	GLU
1	A	521	VAL
1	A	596	VAL
1	A	597	VAL
1	A	606	GLU
1	A	844	VAL
1	A	868	HIS
1	A	869	GLN
1	A	925	MET
1	A	969	MET
1	A	992	LEU
1	A	993	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	138	GLN
1	A	768	ASN
1	A	919	ASN
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 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	1.72	4 (15%)
2	1HT	A	1001	-	50,53,53	3.21	22 (44%)	57,78,78	3.56	31 (54%)

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	-	-	8/27/27/53	-
2	1HT	A	1001	-	-	18/41/107/107	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	1HT	OAO-CBP	7.33	1.36	1.20
3	A	1002	PTY	O30-C30	7.07	1.43	1.22
2	A	1001	1HT	OBG-CBX	-6.96	1.36	1.48
2	A	1001	1HT	CBW-CBY	-6.79	1.46	1.55
2	A	1001	1HT	OBD-CBT	-6.72	1.34	1.44
2	A	1001	1HT	OBC-CBR	-6.21	1.36	1.46
2	A	1001	1HT	OBE-CBS	-5.68	1.34	1.44
2	A	1001	1HT	OBF-CBU	-5.65	1.37	1.46
2	A	1001	1HT	OBF-CBP	5.09	1.42	1.35
2	A	1001	1HT	CAQ-CBJ	4.92	1.60	1.31
2	A	1001	1HT	CBN-CBQ	4.69	1.54	1.33
2	A	1001	1HT	CAG-CBN	-4.41	1.43	1.50
2	A	1001	1HT	CBY-CBU	-4.10	1.47	1.53
2	A	1001	1HT	OBE-CBO	3.88	1.43	1.34
2	A	1001	1HT	CAF-CBJ	3.78	1.59	1.50
2	A	1001	1HT	CBS-CBN	3.77	1.55	1.50
2	A	1001	1HT	CBO-CBJ	3.73	1.62	1.50
3	A	1002	PTY	O4-C30	3.60	1.43	1.33
2	A	1001	1HT	OBH-CBY	-2.69	1.40	1.44
2	A	1001	1HT	CBY-CBR	2.62	1.58	1.52
2	A	1001	1HT	OBH-CBM	2.61	1.41	1.33
2	A	1001	1HT	OBC-CBK	2.60	1.41	1.34
2	A	1001	1HT	OAP-CBW	-2.52	1.38	1.42
2	A	1001	1HT	CBB-CBX	-2.24	1.50	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	1HT	OBF-CBP-OAO	-13.27	104.43	121.60
2	A	1001	1HT	CAG-CBN-CBQ	-10.50	103.88	130.03
2	A	1001	1HT	OAO-CBP-CBW	-9.10	119.08	128.28
2	A	1001	1HT	CBU-OBF-CBP	-6.27	102.10	110.80
3	A	1002	PTY	O4-C30-O30	-6.07	108.45	123.63
2	A	1001	1HT	CBB-CBR-CBY	5.78	122.70	115.35
2	A	1001	1HT	CBY-CBU-CBQ	5.36	129.00	115.29
2	A	1001	1HT	CBY-OBH-CBM	5.20	131.51	119.93
3	A	1002	PTY	O30-C30-C31	-4.01	108.09	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	1HT	OBH-CBM-OAM	-3.95	115.81	125.08
2	A	1001	1HT	OBE-CBO-CBJ	3.70	121.16	111.46
2	A	1001	1HT	CBX-OBG-CBI	3.30	129.08	121.36
2	A	1001	1HT	CAF-CBJ-CAQ	-3.28	110.55	123.12
2	A	1001	1HT	CBX-CBV-CBQ	-3.26	110.64	115.07
2	A	1001	1HT	OBH-CBM-CAZ	3.10	116.08	110.67
2	A	1001	1HT	CAG-CBN-CBS	-3.09	116.10	121.24
2	A	1001	1HT	OBF-CBU-CBQ	3.08	115.73	111.17
2	A	1001	1HT	CBS-CBN-CBQ	-2.99	96.98	108.36
2	A	1001	1HT	OBC-CBK-OAK	-2.97	116.75	123.70
2	A	1001	1HT	OBG-CBI-OAJ	-2.92	118.53	123.61
2	A	1001	1HT	OBG-CBI-CAE	2.79	115.41	110.67
2	A	1001	1HT	OAM-CBM-CAZ	-2.77	112.93	123.78
2	A	1001	1HT	OBE-CBO-OAN	-2.72	118.32	123.40
3	A	1002	PTY	C6-O7-C8	-2.59	111.60	117.80
2	A	1001	1HT	CBU-CBQ-CBN	-2.47	115.36	126.58
2	A	1001	1HT	OBC-CBR-CBB	2.46	111.03	106.63
2	A	1001	1HT	OAN-CBO-CBJ	-2.40	117.66	125.28
3	A	1002	PTY	O7-C8-C11	2.40	119.75	110.93
2	A	1001	1HT	OBC-CBR-CBY	-2.38	102.04	106.41
2	A	1001	1HT	OAP-CBW-CAH	-2.37	104.88	109.45
2	A	1001	1HT	OBD-CBL-CBA	2.33	116.51	111.48
2	A	1001	1HT	CBW-CBY-CBR	2.27	117.46	114.44
2	A	1001	1HT	CAA-CAQ-CBJ	-2.16	116.05	127.73
2	A	1001	1HT	OAJ-CBI-CAE	-2.07	117.44	124.77
2	A	1001	1HT	OAK-CBK-CAY	-2.02	115.89	123.78

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	CAA-CAQ-CBJ-CBO
2	A	1001	1HT	CAA-CAQ-CBJ-CAF
3	A	1002	PTY	C3-O11-P1-O12
3	A	1002	PTY	O30-C30-O4-C1
2	A	1001	1HT	OAN-CBO-OBE-CBS
2	A	1001	1HT	CAF-CBJ-CBO-OAN
3	A	1002	PTY	C31-C30-O4-C1

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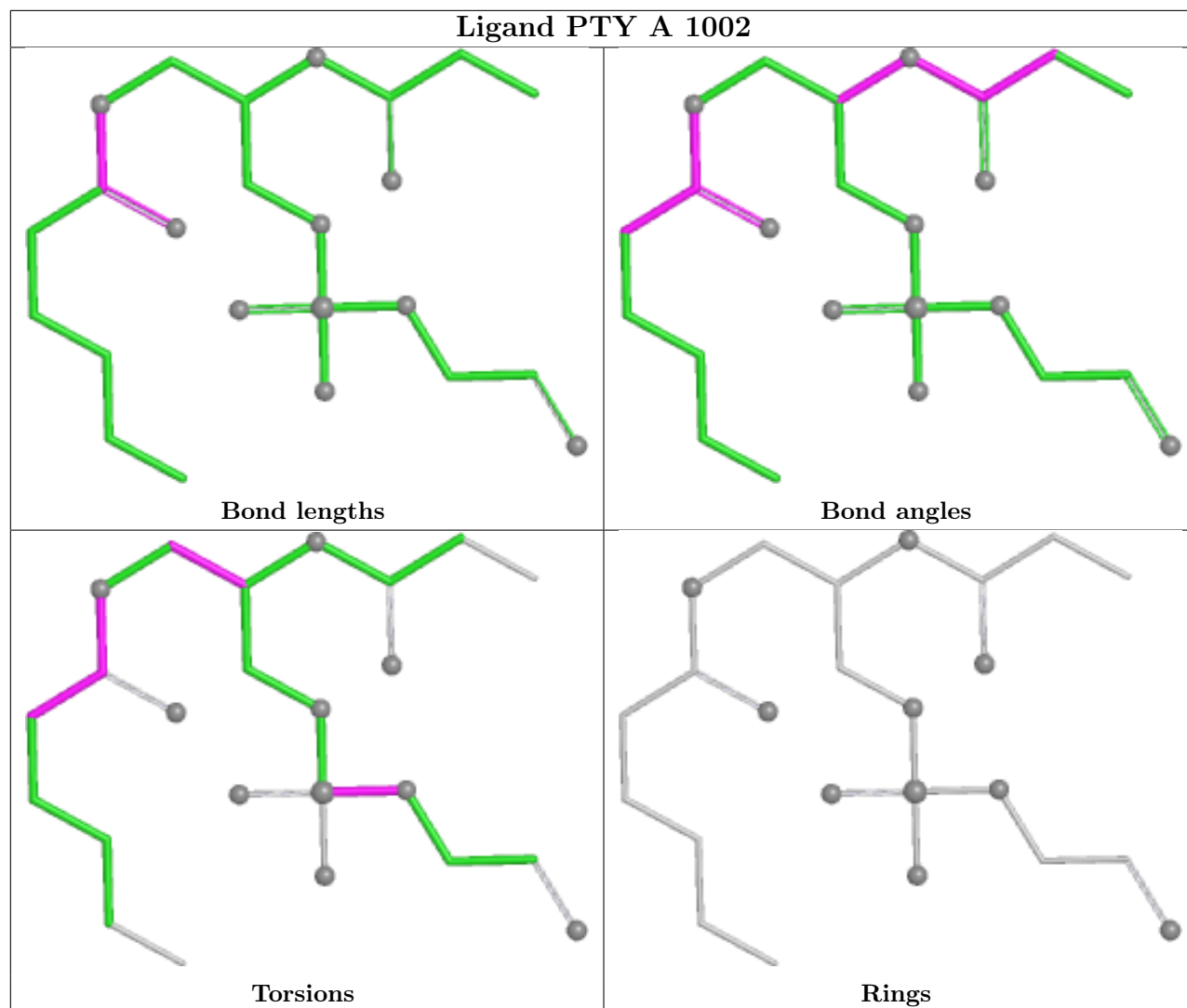
Mol	Chain	Res	Type	Atoms
2	A	1001	1HT	OAJ-CBI-OBG-CBX
3	A	1002	PTY	O4-C1-C6-O7
2	A	1001	1HT	OAK-CBK-OBC-CBR
2	A	1001	1HT	CBJ-CBO-OBE-CBS
2	A	1001	1HT	CAU-CAV-CAW-CAX
2	A	1001	1HT	CBA-CBL-OBDB-CBT
2	A	1001	1HT	CAB-CAR-CAU-CAV
2	A	1001	1HT	CAW-CAX-CBA-CBL
3	A	1002	PTY	O4-C1-C6-C5
3	A	1002	PTY	C3-O11-P1-O13
3	A	1002	PTY	C3-O11-P1-O14
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

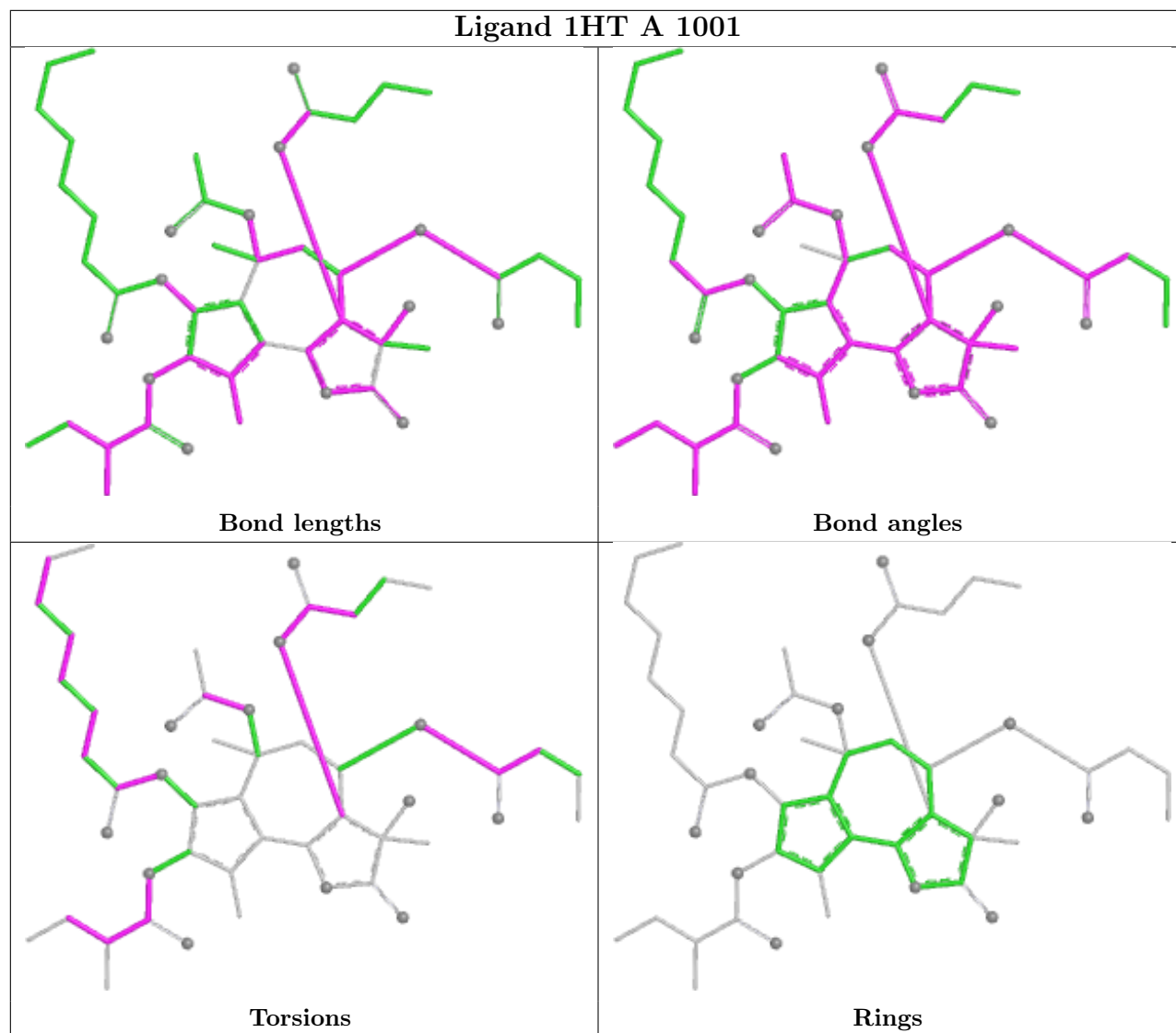
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	PTY	4	0
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 [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%)	0.18	18 (1%)	67 48	30, 91, 164, 257	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	LEU	3.7
1	A	48	SER	3.4
1	A	420	CYS	3.2
1	A	377	CYS	2.9
1	A	81	GLY	2.7
1	A	404	SER	2.7
1	A	50	TRP	2.5
1	A	578	LEU	2.5
1	A	503	SER	2.4
1	A	964	LEU	2.4
1	A	289	ILE	2.4
1	A	1	MET	2.4
1	A	888	CYS	2.4
1	A	31	ARG	2.3
1	A	26	PRO	2.2
1	A	981	ASP	2.2
1	A	293	ILE	2.1
1	A	799	THR	2.1

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

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

6.3 Carbohydrates [i](#)

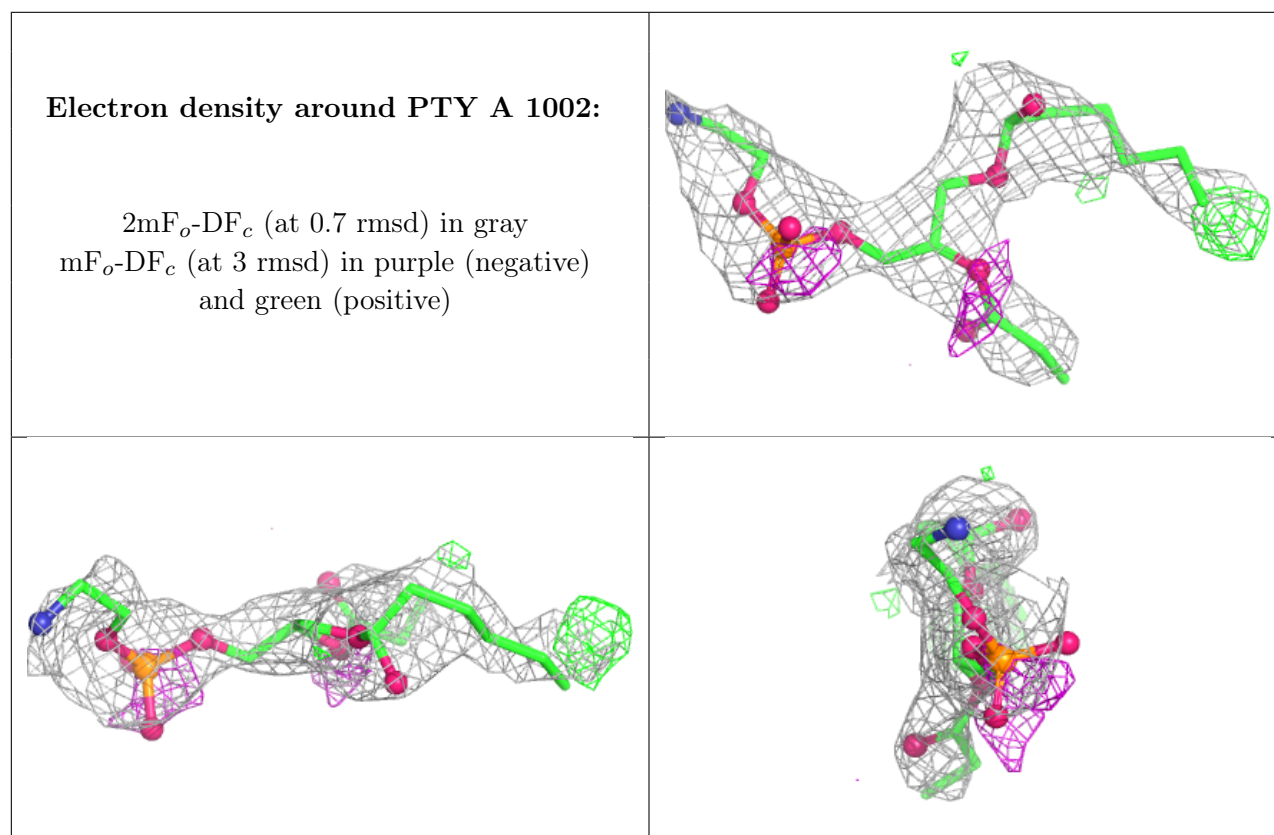
There are no oligosaccharides in this entry.

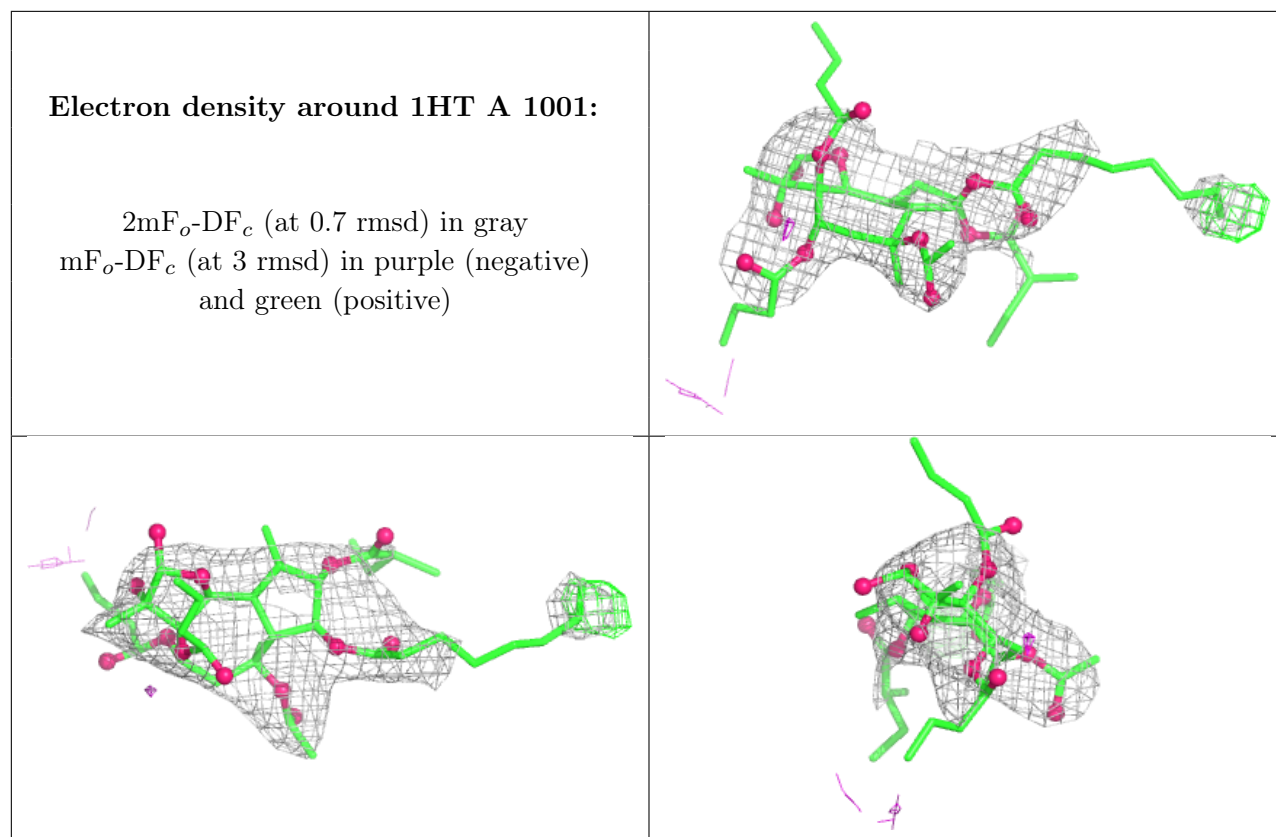
6.4 Ligands [i](#)

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	PTY	A	1002	24/50	0.70	0.21	114,124,132,133	0
2	1HT	A	1001	51/51	0.87	0.20	152,152,152,152	0
4	K	A	1003	1/1	0.93	0.06	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.