WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2025 – 04:19 AM EDT

PDB ID	:	3NAM / pdb_00003nam
Title	:	SR Ca(2+)-ATPase in the HnE2 state complexed with the Thapsigargin derivative dOTg
Authors	:	Winther, A.M.L.; Sonntag, Y.; Olesen, C.; Moller, J.V.; Nissen, P.
Deposited on	:	2010-06-02
Resolution	:	3.10 Å(reported)

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

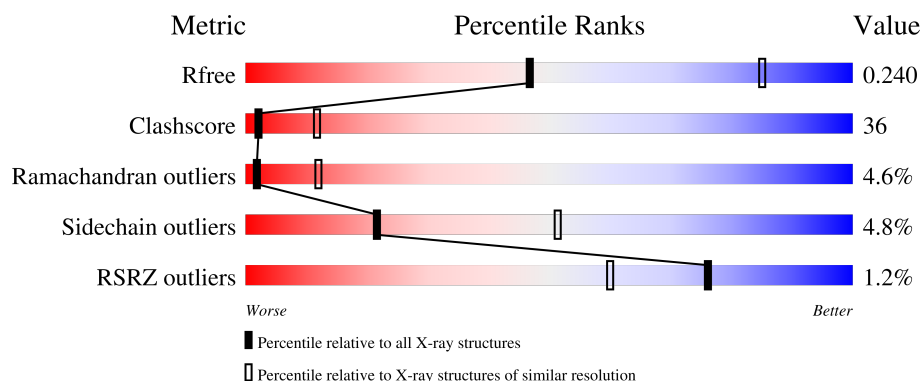|		
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.240
Clashscore		36
Ramachandran outliers		4.6%
Sidechain outliers		4.8%
RSRZ outliers		1.2%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	45% 47% 7% •

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7736 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
1	A	994	Total 7671	C 4876	N 1287	O 1451	S 57	0	0	0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is (3S,3aR,4S,6S,6aS,8R,9R,9aR,9bS)-6-(acetyloxy)-4-(butanoyloxy)-3,3a-dihydroxy-3,6,9-trimethyl-2-oxododecahydroazuleno[4,5-b]furan-8-yl (2Z)-2-methylbut-2-enoate (CCD ID: OTK) (formula: $C_{26}H_{38}O_{10}$).
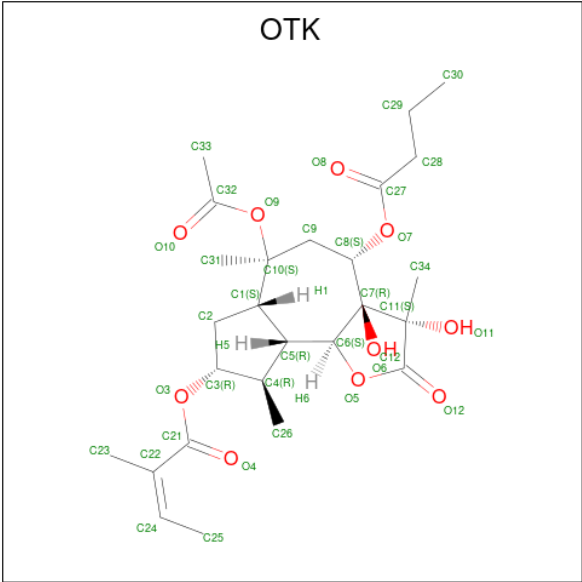
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 36	C 26	O 10	0	0

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).
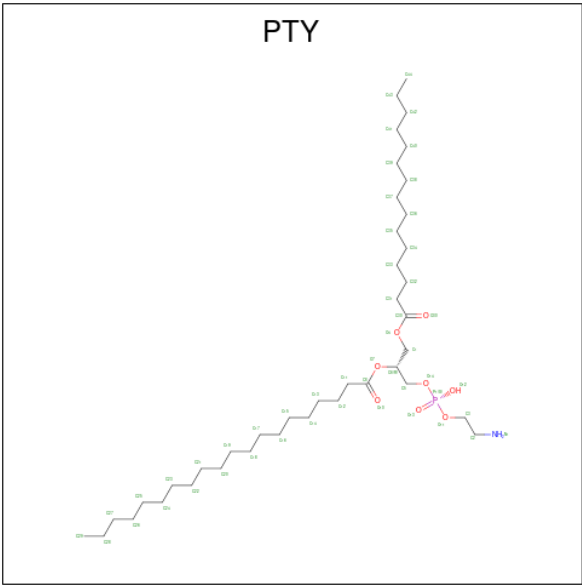
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 24	C 14	N 1	O 8	P 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: SERCA1a
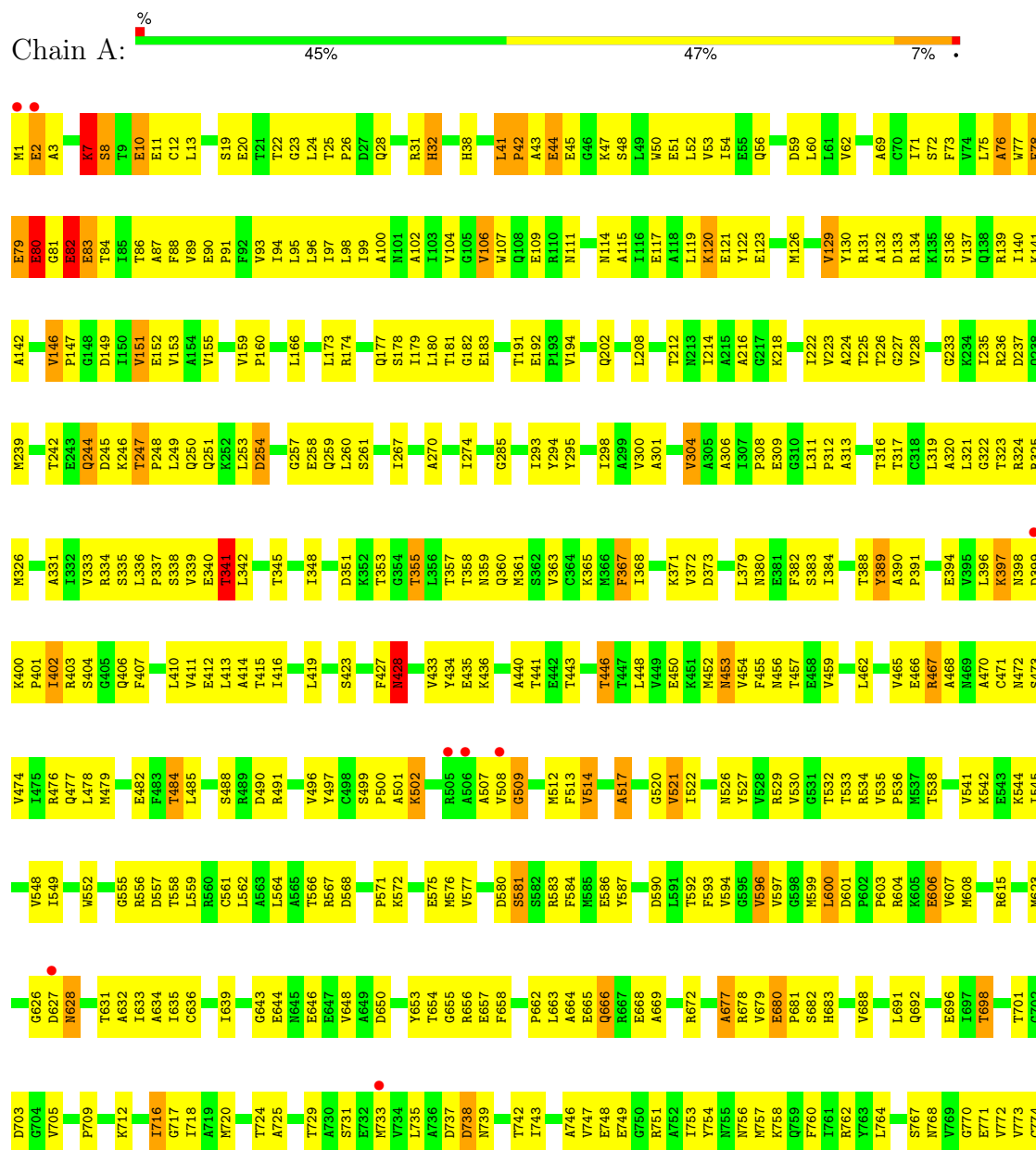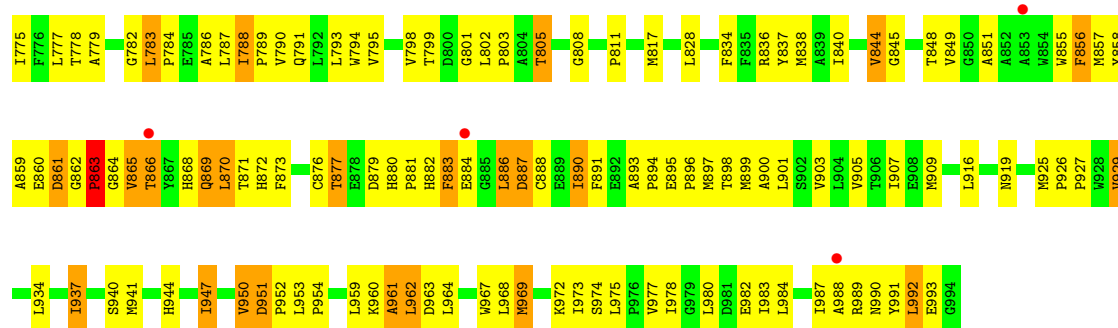
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	71.55Å 71.55Å 591.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10	Depositor
	30.00 – 3.10	EDS
% Data completeness	88.4 (30.00-3.10)	Depositor
(in resolution range)	88.2 (30.00-3.10)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.11Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.280	Depositor
	0.232 , 0.240	DCC
R_{free} test set	825 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å^2)	100.1	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.5	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7736	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, PTY, NA, OTK

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	0.64	7/7812 (0.1%)	1.09	41/10592 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	LYS	CA-C	-5.55	1.45	1.52
1	A	244	GLN	CD-OE1	5.29	1.33	1.23
1	A	32	HIS	ND1-CE1	5.27	1.37	1.32
1	A	608	MET	SD-CE	5.26	1.92	1.79
1	A	38	HIS	ND1-CE1	5.26	1.37	1.32
1	A	666	GLN	CD-OE1	5.24	1.33	1.23
1	A	428	ASN	CG-OD1	5.04	1.33	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	870	LEU	N-CA-C	-8.85	102.48	113.28
1	A	632	ALA	N-CA-C	-8.53	101.94	111.07
1	A	925	MET	CA-C-N	7.17	124.89	119.66
1	A	925	MET	C-N-CA	7.17	124.89	119.66
1	A	194	VAL	CA-C-N	7.15	127.47	119.32
1	A	194	VAL	C-N-CA	7.15	127.47	119.32
1	A	389	TYR	N-CA-C	-6.97	104.52	113.16
1	A	532	THR	N-CA-C	-6.90	104.38	114.39
1	A	435	GLU	N-CA-C	6.77	119.55	108.52
1	A	7	LYS	CA-C-N	-6.71	108.72	121.54
1	A	7	LYS	C-N-CA	-6.71	108.72	121.54
1	A	517	ALA	CA-C-N	6.65	125.89	118.97
1	A	517	ALA	C-N-CA	6.65	125.89	118.97
1	A	309	GLU	N-CA-C	6.61	119.48	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	38	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	A	628	ASN	N-CA-C	-6.43	102.04	110.33
1	A	351	ASP	N-CA-C	-6.18	101.33	110.48
1	A	32	HIS	CB-CG-CD2	-6.16	123.20	131.20
1	A	838	MET	N-CA-C	-6.11	104.70	111.36
1	A	499	SER	N-CA-C	-6.06	102.46	110.40
1	A	716	ILE	CB-CA-C	-6.06	103.52	110.73
1	A	80	GLU	N-CA-C	-6.00	98.03	110.80
1	A	514	VAL	N-CA-C	5.91	117.10	108.53
1	A	926	PRO	N-CA-C	5.79	116.03	110.47
1	A	561	CYS	N-CA-C	5.73	118.97	109.46
1	A	38	HIS	CB-CG-ND1	5.64	131.15	122.70
1	A	254	ASP	N-CA-C	-5.63	105.14	112.23
1	A	348	ILE	CB-CA-C	-5.50	104.19	110.73
1	A	615	ARG	N-CA-C	-5.46	105.23	111.07
1	A	41	LEU	N-CA-C	-5.39	101.81	109.62
1	A	32	HIS	CB-CG-ND1	5.38	130.77	122.70
1	A	446	THR	N-CA-C	-5.34	105.54	111.36
1	A	600	LEU	N-CA-C	5.30	118.09	109.24
1	A	7	LYS	CB-CA-C	-5.26	99.95	110.42
1	A	208	LEU	N-CA-C	-5.16	101.28	109.59
1	A	194	VAL	N-CA-C	-5.13	102.11	107.60
1	A	969	MET	N-CA-C	-5.12	105.78	111.36
1	A	698	THR	N-CA-C	5.10	117.81	109.59
1	A	44	GLU	N-CA-C	5.09	117.02	109.69
1	A	798	VAL	N-CA-C	5.07	119.89	109.34
1	A	869	GLN	N-CA-C	5.01	117.44	108.17

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	7766	557	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	36	0	38	11	0
5	A	24	0	21	2	0
6	A	3	0	0	0	0
All	All	7736	0	7825	566	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 (566) 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:950:VAL:HG12	1:A:951:ASP:H	1.00	1.10
1:A:654:THR:HG22	1:A:657:GLU:HG3	1.40	1.03
1:A:371:LYS:HE2	1:A:373:ASP:HB2	1.42	1.02
1:A:863:PRO:HG2	1:A:890:ILE:HG21	1.41	1.01
1:A:668:GLU:HG3	1:A:672:ARG:HH12	1.20	1.01
1:A:298:ILE:CD1	1:A:779:ALA:HB2	1.92	0.97
1:A:331:ALA:HB1	1:A:733:MET:HE2	1.45	0.94
1:A:950:VAL:HG12	1:A:951:ASP:N	1.77	0.94
1:A:950:VAL:CG1	1:A:951:ASP:H	1.79	0.94
1:A:909:MET:HE3	1:A:937:ILE:HG12	1.49	0.93
1:A:680:GLU:HB2	1:A:681:PRO:HD2	1.49	0.92
1:A:865:VAL:HA	1:A:868:HIS:CE1	2.04	0.92
1:A:927:PRO:HB2	1:A:934:LEU:HD21	1.53	0.90
1:A:77:TRP:HD1	1:A:88:PHE:CZ	1.90	0.89
1:A:876:CYS:CB	1:A:888:CYS:SG	2.60	0.89
1:A:19:SER:OG	1:A:22:THR:HB	1.73	0.88
1:A:77:TRP:HD1	1:A:88:PHE:HZ	1.18	0.88
1:A:527:TYR:HB2	1:A:592:THR:HG22	1.57	0.87
1:A:248:PRO:HD2	1:A:341:THR:HG23	1.55	0.86
1:A:876:CYS:HB2	1:A:888:CYS:SG	2.15	0.86
1:A:77:TRP:CD1	1:A:88:PHE:HZ	1.94	0.86
1:A:397:LYS:HB2	1:A:402:ILE:CD1	2.06	0.86
1:A:788:ILE:HG23	1:A:789:PRO:HD2	1.57	0.85
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.57	0.85
1:A:748:GLU:HA	1:A:817:MET:HE3	1.56	0.85
1:A:153:VAL:HB	1:A:214:ILE:CD1	2.07	0.84
1:A:7:LYS:O	1:A:8:SER:HB3	1.76	0.84
1:A:312:PRO:O	1:A:316:THR:HG23	1.78	0.84
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:THR:HG22	1:A:389:TYR:H	1.44	0.83
1:A:1:MET:HA	1:A:224:ALA:O	1.79	0.83
1:A:557:ASP:HB3	1:A:559:LEU:HG	1.61	0.83
1:A:247:THR:HG23	1:A:250:GLN:HG3	1.59	0.82
1:A:50:TRP:O	1:A:54:ILE:HG12	1.80	0.82
1:A:59:ASP:HB3	1:A:62:VAL:HG12	1.61	0.82
1:A:654:THR:HA	1:A:677:ALA:HB3	1.58	0.82
1:A:319:LEU:HD21	1:A:757:MET:HE1	1.59	0.82
1:A:81:GLY:O	1:A:82:GLU:HB3	1.77	0.82
1:A:876:CYS:HB3	1:A:888:CYS:SG	2.19	0.82
1:A:342:LEU:O	1:A:345:THR:HG23	1.80	0.82
1:A:680:GLU:HB2	1:A:681:PRO:CD	2.10	0.81
1:A:453:ASN:HB3	1:A:471:CYS:SG	2.21	0.81
1:A:394:GLU:OE2	1:A:401:PRO:HB3	1.81	0.81
1:A:801:GLY:O	1:A:805:THR:HG23	1.81	0.80
1:A:751:ARG:HD2	1:A:817:MET:HE2	1.64	0.80
1:A:361:MET:HE3	1:A:599:MET:HE2	1.62	0.80
1:A:791:GLN:HB3	1:A:901:LEU:CD1	2.12	0.79
1:A:865:VAL:HG11	1:A:870:LEU:HB3	1.65	0.79
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.65	0.78
1:A:1:MET:HB2	1:A:225:THR:HG22	1.63	0.78
1:A:855:TRP:CE3	1:A:896:PRO:HG3	2.20	0.77
1:A:522:ILE:HG22	1:A:542:LYS:HE3	1.66	0.76
1:A:77:TRP:CE3	1:A:78:PHE:HB2	2.20	0.76
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.66	0.76
1:A:388:THR:HG22	1:A:389:TYR:N	1.99	0.75
1:A:662:PRO:HG2	1:A:665:GLU:OE1	1.86	0.75
1:A:247:THR:HG23	1:A:250:GLN:CG	2.16	0.75
1:A:545:ILE:O	1:A:549:ILE:HG12	1.87	0.74
1:A:126:MET:HG2	1:A:141:LYS:HA	1.69	0.74
1:A:654:THR:CG2	1:A:657:GLU:HG3	2.16	0.74
1:A:357:THR:HA	1:A:603:PRO:HA	1.70	0.74
1:A:411:VAL:HG22	1:A:454:VAL:CG1	2.19	0.73
1:A:576:MET:HE3	1:A:587:TYR:CD2	2.23	0.73
1:A:397:LYS:HB2	1:A:402:ILE:HD11	1.71	0.73
1:A:530:VAL:O	1:A:530:VAL:HG23	1.87	0.73
1:A:865:VAL:O	1:A:865:VAL:HG12	1.88	0.73
1:A:836:ARG:O	1:A:840:ILE:HG12	1.89	0.73
1:A:879:ASP:C	1:A:881:PRO:HD2	2.14	0.73
1:A:311:LEU:HD13	1:A:764:LEU:HD12	1.70	0.72
1:A:319:LEU:CD2	1:A:757:MET:HE1	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HB	1:A:214:ILE:HD11	1.68	0.72
1:A:397:LYS:HB2	1:A:402:ILE:HD12	1.71	0.72
1:A:441:THR:HA	1:A:599:MET:HE1	1.71	0.72
1:A:606:GLU:H	1:A:606:GLU:CD	1.95	0.72
1:A:247:THR:HG23	1:A:250:GLN:CD	2.15	0.72
1:A:775:ILE:O	1:A:778:THR:HG22	1.89	0.71
1:A:991:TYR:O	1:A:992:LEU:HB2	1.89	0.71
1:A:52:LEU:HD21	1:A:106:VAL:HA	1.73	0.71
1:A:82:GLU:HG3	1:A:83:GLU:N	2.04	0.70
1:A:239:MET:O	1:A:242:THR:HG22	1.91	0.70
1:A:102:ALA:O	1:A:106:VAL:HG12	1.91	0.70
4:A:997:OTK:O8	4:A:997:OTK:O11	2.09	0.70
1:A:411:VAL:HG22	1:A:454:VAL:HG11	1.72	0.70
1:A:558:THR:HG22	1:A:634:ALA:HB1	1.71	0.70
1:A:270:ALA:O	1:A:274:ILE:HG12	1.91	0.70
1:A:791:GLN:NE2	1:A:959:LEU:HD21	2.06	0.69
1:A:880:HIS:N	1:A:881:PRO:HD2	2.06	0.69
1:A:581:SER:HA	1:A:584:PHE:CD2	2.27	0.69
1:A:668:GLU:HG3	1:A:672:ARG:NH1	2.01	0.69
1:A:331:ALA:HB1	1:A:733:MET:CE	2.20	0.69
1:A:894:PRO:O	1:A:898:THR:HG23	1.92	0.69
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.74	0.69
1:A:436:LYS:HG3	1:A:443:THR:HG21	1.75	0.69
1:A:869:GLN:HB3	1:A:872:HIS:ND1	2.07	0.69
1:A:298:ILE:HD13	1:A:779:ALA:HB2	1.74	0.68
1:A:751:ARG:HD2	1:A:817:MET:CE	2.23	0.68
1:A:648:VAL:HG12	1:A:648:VAL:O	1.93	0.68
1:A:131:ARG:NH1	1:A:149:ASP:OD2	2.26	0.68
1:A:988:ALA:HA	1:A:992:LEU:HD23	1.75	0.68
1:A:25:THR:HA	1:A:132:ALA:HB3	1.75	0.67
1:A:300:VAL:O	1:A:304:VAL:HG13	1.94	0.67
1:A:478:LEU:HD23	1:A:479:MET:HG2	1.76	0.67
1:A:748:GLU:HA	1:A:817:MET:CE	2.23	0.67
1:A:7:LYS:O	1:A:8:SER:CB	2.40	0.67
1:A:22:THR:HG22	1:A:132:ALA:HB2	1.75	0.67
1:A:89:VAL:O	1:A:93:VAL:HG23	1.95	0.67
1:A:535:VAL:HG12	1:A:536:PRO:CD	2.25	0.66
1:A:836:ARG:HG2	1:A:984:LEU:HD13	1.75	0.66
1:A:192:GLU:OE1	1:A:580:ASP:HB2	1.95	0.66
1:A:969:MET:O	1:A:973:ILE:HG13	1.95	0.66
1:A:758:LYS:HG3	1:A:828:LEU:CD2	2.26	0.66

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:ALA:O	1:A:729:THR:HG23	1.96	0.65
1:A:471:CYS:O	1:A:474:VAL:HG22	1.96	0.65
1:A:898:THR:HG21	1:A:960:LYS:H	1.61	0.65
1:A:79:GLU:O	1:A:80:GLU:HB2	1.97	0.65
1:A:748:GLU:OE2	1:A:817:MET:HG3	1.96	0.65
1:A:863:PRO:HG2	1:A:890:ILE:CG2	2.24	0.64
1:A:791:GLN:NE2	1:A:897:MET:HE2	2.13	0.64
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.78	0.64
1:A:472:ASN:O	1:A:476:ARG:HG3	1.97	0.64
1:A:688:VAL:O	1:A:692:GLN:HG3	1.98	0.64
1:A:173:LEU:HD12	1:A:216:ALA:O	1.98	0.64
1:A:535:VAL:HG12	1:A:536:PRO:HD2	1.80	0.64
1:A:32:HIS:CB	1:A:146:VAL:HG11	2.28	0.63
1:A:572:LYS:HB2	1:A:575:GLU:HG2	1.80	0.63
1:A:654:THR:HG22	1:A:657:GLU:CG	2.24	0.63
1:A:757:MET:HA	1:A:760:PHE:CE2	2.33	0.63
1:A:81:GLY:O	1:A:82:GLU:O	2.16	0.63
1:A:427:PHE:HB3	1:A:465:VAL:HA	1.80	0.63
1:A:691:LEU:O	1:A:696:GLU:HB2	1.98	0.63
1:A:549:ILE:HD11	1:A:596:VAL:HG11	1.80	0.63
1:A:916:LEU:CD1	1:A:927:PRO:HA	2.29	0.63
1:A:60:LEU:HD21	1:A:261:SER:HB2	1.80	0.62
1:A:436:LYS:CG	1:A:443:THR:HG21	2.29	0.62
1:A:313:ALA:O	1:A:317:THR:HG23	2.00	0.62
1:A:600:LEU:HD12	1:A:601:ASP:N	2.14	0.61
1:A:788:ILE:HG23	1:A:789:PRO:CD	2.29	0.61
1:A:82:GLU:O	1:A:83:GLU:HB3	2.00	0.61
1:A:99:ILE:HG13	1:A:100:ALA:N	2.15	0.61
1:A:183:GLU:OE2	1:A:202:GLN:HG3	2.00	0.61
1:A:654:THR:HG23	1:A:656:ARG:H	1.66	0.61
1:A:857:MET:HG2	1:A:865:VAL:HB	1.80	0.61
1:A:87:ALA:O	1:A:88:PHE:HB2	1.98	0.61
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.30	0.61
1:A:623:MET:HE1	1:A:635:ILE:HG22	1.81	0.61
1:A:249:LEU:HB2	1:A:340:GLU:OE1	2.00	0.61
1:A:1:MET:O	1:A:2:GLU:HB3	2.00	0.61
1:A:25:THR:HB	1:A:26:PRO:HD2	1.82	0.61
1:A:404:SER:OG	1:A:452:MET:HB2	2.00	0.61
1:A:69:ALA:HB2	1:A:94:ILE:HG21	1.83	0.61
1:A:95:LEU:O	1:A:99:ILE:HG12	2.00	0.60
1:A:865:VAL:HG22	1:A:868:HIS:NE2	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:THR:HG22	1:A:657:GLU:H	1.64	0.60
1:A:865:VAL:HG13	1:A:868:HIS:CD2	2.36	0.60
1:A:259:GLN:C	1:A:261:SER:H	2.10	0.60
1:A:861:ASP:CG	1:A:861:ASP:O	2.45	0.60
1:A:969:MET:HE3	1:A:973:ILE:HD11	1.82	0.60
1:A:22:THR:HG22	1:A:132:ALA:CB	2.31	0.60
1:A:301:ALA:HB1	1:A:775:ILE:HD12	1.84	0.60
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.42	0.60
1:A:748:GLU:HG3	1:A:817:MET:HE3	1.83	0.60
1:A:882:HIS:O	1:A:883:PHE:C	2.45	0.60
1:A:361:MET:CE	1:A:599:MET:HE2	2.29	0.59
1:A:848:THR:HA	1:A:903:VAL:HG11	1.83	0.59
1:A:76:ALA:O	1:A:87:ALA:HB1	2.02	0.59
1:A:909:MET:CE	1:A:937:ILE:HA	2.33	0.59
1:A:407:PHE:O	1:A:411:VAL:HG23	2.01	0.59
1:A:90:GLU:OE2	1:A:789:PRO:HG2	2.01	0.59
1:A:114:ASN:HB3	1:A:117:GLU:HG2	1.84	0.59
1:A:500:PRO:HG3	1:A:509:GLY:HA2	1.84	0.59
1:A:32:HIS:HB3	1:A:146:VAL:HG11	1.85	0.59
1:A:73:PHE:HA	1:A:91:PRO:HG2	1.85	0.59
1:A:367:PHE:CD1	1:A:367:PHE:C	2.81	0.59
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.85	0.59
1:A:23:GLY:HA3	1:A:130:TYR:O	2.02	0.58
1:A:96:LEU:O	1:A:100:ALA:HB3	2.04	0.58
1:A:398:ASN:C	1:A:400:LYS:H	2.12	0.58
1:A:77:TRP:CD1	1:A:88:PHE:CZ	2.77	0.58
1:A:359:ASN:N	1:A:601:ASP:OD1	2.36	0.58
1:A:433:VAL:HG12	1:A:434:TYR:N	2.18	0.58
1:A:650:ASP:HB3	1:A:672:ARG:HE	1.69	0.58
1:A:388:THR:CG2	1:A:389:TYR:H	2.15	0.58
1:A:383:SER:C	1:A:384:ILE:HD12	2.29	0.57
1:A:988:ALA:HA	1:A:992:LEU:CD2	2.34	0.57
1:A:19:SER:HG	1:A:22:THR:HB	1.67	0.57
1:A:179:ILE:HG13	1:A:180:LEU:N	2.19	0.57
1:A:398:ASN:O	1:A:399:ASP:HB2	2.03	0.57
1:A:32:HIS:HB3	1:A:146:VAL:CG1	2.35	0.57
1:A:358:THR:HG22	1:A:360:GLN:HB2	1.85	0.57
1:A:179:ILE:O	1:A:705:VAL:HG12	2.05	0.56
1:A:192:GLU:CD	1:A:580:ASP:HB2	2.30	0.56
1:A:462:LEU:HD13	1:A:466:GLU:OE1	2.05	0.56
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:VAL:HA	1:A:868:HIS:HE1	1.64	0.56
1:A:733:MET:HE1	1:A:746:ALA:HB1	1.86	0.56
1:A:863:PRO:CG	1:A:890:ILE:HG21	2.26	0.56
1:A:115:ALA:HB1	1:A:239:MET:HE1	1.87	0.56
1:A:177:GLN:HB3	1:A:212:THR:HG21	1.88	0.56
1:A:88:PHE:C	1:A:91:PRO:HD2	2.30	0.56
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.40	0.56
1:A:907:ILE:HG23	1:A:977:VAL:HG21	1.87	0.56
1:A:367:PHE:CD2	1:A:596:VAL:HG22	2.41	0.56
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.41	0.56
1:A:703:ASP:O	1:A:724:THR:HG23	2.06	0.56
1:A:879:ASP:OD1	1:A:882:HIS:HB3	2.05	0.55
1:A:402:ILE:CG2	1:A:403:ARG:N	2.69	0.55
1:A:791:GLN:HE21	1:A:959:LEU:HD21	1.71	0.55
1:A:909:MET:HE3	1:A:937:ILE:CG1	2.27	0.55
1:A:44:GLU:HG3	1:A:117:GLU:OE2	2.07	0.55
1:A:811:PRO:HG2	1:A:929:VAL:CG1	2.37	0.55
1:A:317:THR:O	1:A:321:LEU:HG	2.07	0.55
4:A:997:OTK:O6	4:A:997:OTK:H1	2.06	0.55
1:A:50:TRP:CZ2	1:A:54:ILE:HD11	2.41	0.55
1:A:181:THR:OG1	1:A:183:GLU:HG3	2.07	0.55
1:A:249:LEU:CB	1:A:340:GLU:OE1	2.55	0.55
1:A:623:MET:HE1	1:A:635:ILE:CG2	2.37	0.55
1:A:718:ILE:CG2	1:A:735:LEU:HG	2.37	0.54
1:A:382:PHE:CE2	1:A:410:LEU:HD11	2.42	0.54
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.38	0.54
1:A:380:ASN:HB3	1:A:382:PHE:HE1	1.73	0.54
1:A:680:GLU:CB	1:A:681:PRO:HD2	2.31	0.54
1:A:52:LEU:HD22	1:A:106:VAL:HB	1.90	0.54
1:A:784:PRO:HG3	1:A:873:PHE:CD2	2.43	0.54
1:A:855:TRP:CZ3	1:A:896:PRO:HG3	2.43	0.54
1:A:82:GLU:O	1:A:83:GLU:CB	2.56	0.53
1:A:126:MET:HA	1:A:142:ALA:H	1.71	0.53
1:A:75:LEU:C	1:A:77:TRP:H	2.16	0.53
1:A:450:GLU:OE1	1:A:467:ARG:NH1	2.41	0.53
1:A:488:SER:OG	1:A:491:ARG:NH1	2.42	0.53
1:A:107:TRP:CE2	1:A:111:ASN:ND2	2.76	0.53
1:A:119:LEU:O	1:A:121:GLU:N	2.41	0.53
1:A:701:THR:HB	1:A:720:MET:CE	2.39	0.53
1:A:391:PRO:HD2	1:A:434:TYR:CE2	2.44	0.53
1:A:836:ARG:HG2	1:A:984:LEU:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TRP:CZ3	1:A:78:PHE:HB2	2.44	0.53
1:A:228:VAL:HG13	1:A:237:ASP:OD2	2.09	0.53
1:A:248:PRO:O	1:A:251:GLN:HB2	2.09	0.53
1:A:59:ASP:HB3	1:A:62:VAL:CG1	2.34	0.53
1:A:60:LEU:HD21	1:A:261:SER:CB	2.38	0.53
1:A:717:GLY:O	1:A:731:SER:HB2	2.08	0.53
1:A:416:ILE:HG21	1:A:564:LEU:HB3	1.90	0.52
1:A:680:GLU:CB	1:A:681:PRO:CD	2.86	0.52
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.39	0.52
4:A:997:OTK:H31B	4:A:997:OTK:H4	1.90	0.52
1:A:249:LEU:HB2	1:A:340:GLU:CD	2.33	0.52
1:A:767:SER:O	1:A:771:GLU:HG3	2.09	0.52
1:A:361:MET:HE3	1:A:599:MET:CE	2.38	0.52
1:A:485:LEU:HD22	1:A:584:PHE:CE1	2.43	0.52
1:A:152:GLU:OE2	1:A:218:LYS:HE3	2.09	0.52
1:A:566:THR:HG23	1:A:594:VAL:HG21	1.92	0.52
1:A:791:GLN:HB3	1:A:901:LEU:HD11	1.89	0.52
1:A:898:THR:HG22	1:A:959:LEU:HA	1.91	0.52
1:A:295:TYR:O	1:A:298:ILE:HG22	2.08	0.52
1:A:69:ALA:HB2	1:A:94:ILE:CG2	2.39	0.52
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.91	0.52
1:A:384:ILE:HD12	1:A:384:ILE:N	2.25	0.52
1:A:558:THR:HG22	1:A:634:ALA:CB	2.40	0.52
1:A:253:LEU:HD23	1:A:253:LEU:O	2.10	0.51
1:A:526:ASN:OD1	1:A:590:ASP:HA	2.10	0.51
1:A:94:ILE:O	1:A:98:LEU:HG	2.10	0.51
1:A:791:GLN:HE22	1:A:897:MET:HE2	1.75	0.51
1:A:254:ASP:O	1:A:258:GLU:HG2	2.11	0.51
1:A:466:GLU:CD	1:A:466:GLU:C	2.78	0.51
1:A:501:ALA:O	1:A:502:LYS:HB2	2.11	0.51
1:A:626:GLY:O	1:A:678:ARG:HG2	2.10	0.51
1:A:631:THR:O	1:A:635:ILE:HG13	2.10	0.51
1:A:388:THR:HG22	1:A:390:ALA:H	1.76	0.51
1:A:541:VAL:O	1:A:545:ILE:HG13	2.11	0.51
1:A:79:GLU:O	1:A:80:GLU:CB	2.57	0.51
1:A:470:ALA:O	1:A:474:VAL:HG13	2.10	0.51
1:A:333:VAL:HG22	1:A:733:MET:HE3	1.92	0.51
1:A:465:VAL:HG23	1:A:466:GLU:N	2.25	0.51
1:A:86:THR:O	1:A:87:ALA:C	2.52	0.51
1:A:916:LEU:HD11	1:A:927:PRO:HA	1.91	0.51
1:A:749:GLU:O	1:A:753:ILE:HG12	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:CYS:SG	1:A:884:GLU:CD	2.94	0.51
1:A:236:ARG:O	1:A:236:ARG:HG2	2.10	0.51
1:A:777:LEU:HB2	1:A:849:VAL:HG21	1.92	0.51
1:A:840:ILE:O	1:A:844:VAL:HG13	2.11	0.50
1:A:83:GLU:HG3	1:A:84:THR:HG23	1.92	0.50
1:A:367:PHE:HA	1:A:380:ASN:O	2.10	0.50
1:A:758:LYS:O	1:A:762:ARG:HG3	2.11	0.50
1:A:783:LEU:HD12	1:A:871:THR:HG22	1.94	0.50
1:A:909:MET:HE3	1:A:937:ILE:HA	1.92	0.50
1:A:535:VAL:CG1	1:A:536:PRO:CD	2.90	0.50
1:A:865:VAL:O	1:A:866:THR:C	2.53	0.50
1:A:109:GLU:C	1:A:109:GLU:OE1	2.54	0.50
1:A:326:MET:HE2	1:A:749:GLU:HB3	1.94	0.50
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.93	0.50
1:A:7:LYS:HB3	1:A:11:GLU:HB2	1.93	0.50
1:A:53:VAL:O	1:A:56:GLN:HB2	2.12	0.50
1:A:121:GLU:C	1:A:121:GLU:CD	2.80	0.50
1:A:581:SER:HA	1:A:584:PHE:CG	2.46	0.50
1:A:600:LEU:HD12	1:A:601:ASP:H	1.76	0.50
1:A:22:THR:CG2	1:A:132:ALA:CB	2.89	0.50
1:A:627:ASP:C	1:A:628:ASN:O	2.54	0.50
1:A:760:PHE:CD1	1:A:760:PHE:C	2.89	0.50
1:A:60:LEU:CD2	1:A:261:SER:HB2	2.41	0.50
1:A:77:TRP:HE3	1:A:78:PHE:HB2	1.74	0.50
1:A:87:ALA:O	1:A:88:PHE:CB	2.60	0.50
1:A:248:PRO:CD	1:A:341:THR:HG23	2.35	0.50
1:A:848:THR:HG22	1:A:903:VAL:HG13	1.92	0.50
1:A:325:ARG:HD2	1:A:749:GLU:OE1	2.12	0.50
1:A:414:ALA:HB2	1:A:452:MET:HE2	1.93	0.50
1:A:126:MET:HB3	1:A:140:ILE:O	2.12	0.49
1:A:298:ILE:HD11	1:A:779:ALA:HB2	1.87	0.49
1:A:379:LEU:CD2	1:A:548:VAL:HG21	2.42	0.49
4:A:997:OTK:H31	4:A:997:OTK:O10	2.12	0.49
1:A:104:VAL:HG21	5:A:998:PTY:HC6	1.93	0.49
1:A:28:GLN:HG2	1:A:31:ARG:NH2	2.28	0.49
1:A:246:LYS:O	1:A:247:THR:C	2.56	0.49
1:A:947:ILE:HG22	1:A:953:LEU:HD13	1.95	0.49
1:A:60:LEU:HD23	1:A:257:GLY:O	2.13	0.49
1:A:45:GLU:HG3	1:A:45:GLU:O	2.12	0.49
1:A:259:GLN:C	1:A:261:SER:N	2.68	0.49
1:A:583:ARG:HH11	1:A:583:ARG:HG2	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:MET:CE	1:A:940:SER:HB2	2.42	0.49
4:A:997:OTK:O10	4:A:997:OTK:H9	2.12	0.49
1:A:48:SER:HB3	1:A:51:GLU:HG3	1.94	0.49
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.42	0.49
1:A:628:ASN:OD1	1:A:631:THR:HG23	2.13	0.49
1:A:654:THR:CG2	1:A:657:GLU:H	2.26	0.49
1:A:865:VAL:O	1:A:865:VAL:CG1	2.60	0.49
1:A:962:LEU:HD12	1:A:967:TRP:CD1	2.48	0.49
1:A:147:PRO:HG3	1:A:226:THR:HB	1.95	0.49
1:A:555:GLY:C	1:A:557:ASP:H	2.21	0.49
1:A:121:GLU:CD	1:A:121:GLU:O	2.57	0.48
1:A:134:ARG:HH21	1:A:136:SER:HB2	1.78	0.48
1:A:782:GLY:O	1:A:873:PHE:HE2	1.96	0.48
1:A:880:HIS:HA	1:A:884:GLU:HB2	1.95	0.48
1:A:893:ALA:O	1:A:896:PRO:HD2	2.13	0.48
1:A:758:LYS:HG3	1:A:828:LEU:HD22	1.95	0.48
1:A:455:PHE:HB2	1:A:457:THR:HG23	1.95	0.48
1:A:473:SER:O	1:A:477:GLN:HG3	2.14	0.48
1:A:754:TYR:O	1:A:758:LYS:HB2	2.13	0.48
1:A:772:VAL:HG21	4:A:997:OTK:H23	1.95	0.48
1:A:126:MET:SD	1:A:139:ARG:NH1	2.87	0.48
1:A:394:GLU:CD	1:A:401:PRO:HB3	2.39	0.48
1:A:396:LEU:HD23	1:A:401:PRO:HA	1.95	0.48
1:A:864:GLY:O	1:A:865:VAL:HG23	2.14	0.48
1:A:119:LEU:O	1:A:120:LYS:C	2.57	0.48
1:A:335:SER:OG	1:A:338:SER:HB2	2.13	0.48
1:A:402:ILE:HG22	1:A:403:ARG:N	2.29	0.48
1:A:358:THR:O	1:A:359:ASN:HB3	2.13	0.48
1:A:834:PHE:C	1:A:834:PHE:CD2	2.91	0.48
1:A:452:MET:O	1:A:454:VAL:N	2.47	0.48
1:A:898:THR:HG21	1:A:960:LYS:N	2.27	0.48
1:A:784:PRO:HG2	1:A:856:PHE:HE2	1.79	0.47
1:A:865:VAL:HG21	1:A:870:LEU:HB3	1.95	0.47
1:A:72:SER:OG	1:A:91:PRO:HG3	2.14	0.47
1:A:389:TYR:CE2	1:A:436:LYS:HB2	2.49	0.47
1:A:130:TYR:CE1	1:A:137:VAL:HB	2.49	0.47
1:A:413:LEU:HG	1:A:564:LEU:HD12	1.96	0.47
1:A:433:VAL:CG1	1:A:434:TYR:N	2.76	0.47
1:A:650:ASP:HB3	1:A:672:ARG:NE	2.30	0.47
1:A:960:LYS:O	1:A:961:ALA:C	2.57	0.47
1:A:992:LEU:HD12	1:A:993:GLU:OE1	2.14	0.47

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:CD2	1:A:106:VAL:HA	2.42	0.47
1:A:96:LEU:O	1:A:100:ALA:CB	2.62	0.47
1:A:153:VAL:CB	1:A:214:ILE:HD11	2.40	0.47
1:A:555:GLY:C	1:A:557:ASP:N	2.71	0.47
1:A:555:GLY:O	1:A:557:ASP:N	2.48	0.47
1:A:568:ASP:OD2	1:A:592:THR:HG21	2.13	0.47
1:A:680:GLU:OE2	1:A:682:SER:HB3	2.14	0.47
1:A:811:PRO:HG2	1:A:929:VAL:HG13	1.96	0.47
1:A:155:VAL:HA	1:A:214:ILE:HG22	1.96	0.47
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.77	0.47
1:A:235:ILE:HG23	1:A:709:PRO:HD3	1.95	0.47
1:A:756:ASN:ND2	1:A:808:GLY:O	2.42	0.47
1:A:79:GLU:HB3	1:A:293:ILE:HD11	1.97	0.47
1:A:368:ILE:HD13	1:A:410:LEU:HD23	1.96	0.47
1:A:527:TYR:O	1:A:592:THR:HA	2.14	0.47
1:A:42:PRO:HD3	1:A:228:VAL:HG23	1.96	0.46
1:A:865:VAL:HG13	1:A:868:HIS:CG	2.49	0.46
1:A:535:VAL:HG12	1:A:536:PRO:N	2.30	0.46
1:A:773:VAL:HG12	1:A:845:GLY:HA3	1.96	0.46
1:A:980:LEU:O	1:A:984:LEU:HG	2.15	0.46
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.98	0.46
1:A:361:MET:HB3	1:A:599:MET:HE3	1.97	0.46
1:A:371:LYS:CE	1:A:373:ASP:HB2	2.31	0.46
1:A:391:PRO:HD2	1:A:434:TYR:CD2	2.50	0.46
1:A:662:PRO:O	1:A:664:ALA:N	2.49	0.46
1:A:758:LYS:HG3	1:A:828:LEU:HD21	1.95	0.46
1:A:951:ASP:HB2	1:A:952:PRO:CD	2.38	0.46
1:A:78:PHE:CD2	1:A:79:GLU:CD	2.94	0.46
1:A:93:VAL:O	1:A:97:ILE:HG12	2.16	0.46
1:A:791:GLN:HB3	1:A:901:LEU:HD12	1.94	0.46
1:A:919:ASN:O	1:A:989:ARG:HD3	2.15	0.46
1:A:941:MET:O	1:A:944:HIS:HB3	2.16	0.46
1:A:500:PRO:CG	1:A:509:GLY:HA2	2.46	0.46
1:A:735:LEU:HD11	1:A:743:ILE:CG1	2.46	0.46
1:A:316:THR:HG21	5:A:998:PTY:HC52	1.98	0.46
1:A:466:GLU:O	1:A:468:ALA:N	2.49	0.46
1:A:903:VAL:O	1:A:907:ILE:HG13	2.15	0.46
1:A:880:HIS:N	1:A:881:PRO:CD	2.76	0.46
1:A:121:GLU:C	1:A:123:GLU:H	2.24	0.45
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.97	0.45
1:A:978:ILE:O	1:A:982:GLU:HG2	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HA	1:A:160:PRO:HD3	1.69	0.45
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.97	0.45
1:A:436:LYS:HD2	1:A:440:ALA:HA	1.98	0.45
1:A:484:THR:HB	1:A:496:VAL:HG12	1.99	0.45
1:A:770:GLY:HA3	1:A:844:VAL:HG21	1.98	0.45
1:A:114:ASN:HB3	1:A:117:GLU:CG	2.46	0.45
1:A:119:LEU:C	1:A:121:GLU:N	2.73	0.45
1:A:311:LEU:CD1	1:A:764:LEU:HD12	2.43	0.45
1:A:81:GLY:C	1:A:82:GLU:O	2.60	0.45
1:A:178:SER:O	1:A:182:GLY:N	2.47	0.45
1:A:603:PRO:O	1:A:604:ARG:C	2.59	0.45
1:A:372:VAL:HG23	1:A:530:VAL:HG11	1.98	0.45
1:A:681:PRO:O	1:A:682:SER:C	2.60	0.45
1:A:851:ALA:HB2	1:A:973:ILE:HD13	1.98	0.45
1:A:877:THR:HG23	1:A:888:CYS:CB	2.47	0.45
1:A:301:ALA:CB	1:A:775:ILE:HD12	2.47	0.45
1:A:466:GLU:C	1:A:468:ALA:N	2.75	0.45
1:A:577:VAL:CG2	1:A:583:ARG:HE	2.29	0.45
1:A:837:TYR:HB2	4:A:997:OTK:H33	1.97	0.45
1:A:361:MET:HB3	1:A:599:MET:CE	2.46	0.45
1:A:397:LYS:CB	1:A:402:ILE:HD11	2.44	0.45
1:A:308:PRO:HB3	1:A:768:ASN:OD1	2.17	0.45
1:A:403:ARG:NH2	1:A:456:ASN:CG	2.75	0.45
1:A:71:ILE:O	1:A:75:LEU:HG	2.17	0.44
1:A:355:THR:HG21	1:A:720:MET:CE	2.47	0.44
1:A:517:ALA:O	1:A:521:VAL:HG13	2.18	0.44
1:A:534:ARG:CD	1:A:592:THR:HG21	2.47	0.44
1:A:648:VAL:O	1:A:648:VAL:CG1	2.63	0.44
1:A:747:VAL:O	1:A:747:VAL:HG12	2.17	0.44
1:A:905:VAL:O	1:A:909:MET:HG2	2.17	0.44
1:A:45:GLU:C	1:A:47:LYS:H	2.26	0.44
1:A:900:ALA:HA	1:A:903:VAL:HG12	1.99	0.44
1:A:41:LEU:HD21	1:A:233:GLY:HA2	2.00	0.44
1:A:83:GLU:CG	1:A:84:THR:HG23	2.48	0.44
1:A:99:ILE:CG1	1:A:100:ALA:N	2.80	0.44
1:A:653:TYR:CE2	1:A:669:ALA:HB1	2.53	0.44
1:A:894:PRO:HD2	1:A:895:GLU:OE1	2.17	0.44
1:A:72:SER:HB2	1:A:300:VAL:HG11	2.00	0.44
1:A:654:THR:HG23	1:A:656:ARG:N	2.30	0.44
1:A:81:GLY:O	1:A:82:GLU:CB	2.47	0.44
1:A:411:VAL:O	1:A:415:THR:HG23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ARG:NH1	1:A:571:PRO:HD3	2.33	0.44
1:A:775:ILE:C	1:A:778:THR:HG22	2.42	0.44
1:A:865:VAL:HG13	1:A:868:HIS:CE1	2.52	0.44
1:A:586:GLU:OE1	1:A:586:GLU:HA	2.18	0.44
1:A:860:GLU:OE1	1:A:860:GLU:HA	2.17	0.44
1:A:355:THR:HA	1:A:738:ASP:O	2.17	0.43
1:A:412:GLU:OE1	1:A:529:ARG:NE	2.51	0.43
1:A:522:ILE:CG2	1:A:542:LYS:HE3	2.44	0.43
1:A:895:GLU:N	1:A:896:PRO:CD	2.81	0.43
1:A:367:PHE:CE2	1:A:596:VAL:HG22	2.52	0.43
1:A:490:ASP:OD1	1:A:491:ARG:N	2.43	0.43
1:A:527:TYR:CD2	1:A:592:THR:HG22	2.53	0.43
1:A:32:HIS:HB2	1:A:146:VAL:HG11	2.00	0.43
1:A:864:GLY:C	1:A:865:VAL:HG23	2.42	0.43
1:A:876:CYS:O	1:A:879:ASP:N	2.46	0.43
1:A:298:ILE:HD12	1:A:779:ALA:HB2	1.92	0.43
1:A:633:ILE:O	1:A:636:CYS:HB2	2.19	0.43
1:A:643:GLY:O	1:A:644:GLU:C	2.61	0.43
1:A:658:PHE:CZ	1:A:666:GLN:HG2	2.54	0.43
1:A:737:ASP:C	1:A:739:ASN:N	2.77	0.43
1:A:24:LEU:HG	1:A:149:ASP:HA	2.00	0.43
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.44	0.43
1:A:756:ASN:HB3	1:A:808:GLY:HA2	2.00	0.43
1:A:882:HIS:CD2	1:A:883:PHE:CD2	3.07	0.43
1:A:260:LEU:O	1:A:260:LEU:HG	2.18	0.43
1:A:679:VAL:HB	1:A:683:HIS:HB2	1.99	0.43
1:A:691:LEU:HD23	1:A:691:LEU:HA	1.82	0.43
1:A:851:ALA:HB1	1:A:899:MET:HE3	1.99	0.43
1:A:900:ALA:O	1:A:903:VAL:HG12	2.18	0.43
1:A:968:LEU:O	1:A:972:LYS:HG3	2.18	0.43
1:A:604:ARG:HD3	1:A:739:ASN:CG	2.43	0.43
1:A:855:TRP:CA	1:A:859:ALA:HB2	2.48	0.43
1:A:873:PHE:HB2	1:A:891:PHE:CG	2.54	0.43
1:A:886:LEU:HD12	1:A:887:ASP:N	2.34	0.43
1:A:898:THR:OG1	1:A:962:LEU:HD23	2.18	0.43
1:A:133:ASP:O	1:A:133:ASP:CG	2.62	0.43
1:A:388:THR:CG2	1:A:389:TYR:N	2.69	0.43
4:A:997:OTK:H4	4:A:997:OTK:C31	2.48	0.43
1:A:10:GLU:C	1:A:12:CYS:N	2.74	0.43
1:A:178:SER:HB3	1:A:183:GLU:O	2.19	0.43
1:A:301:ALA:HB1	1:A:775:ILE:CD1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LEU:HD11	1:A:544:LYS:HG3	2.01	0.43
1:A:655:GLY:HA3	1:A:678:ARG:O	2.19	0.43
1:A:862:GLY:O	1:A:863:PRO:C	2.62	0.43
1:A:882:HIS:CD2	1:A:883:PHE:HD2	2.37	0.43
1:A:530:VAL:O	1:A:530:VAL:CG2	2.60	0.43
1:A:294:TYR:HD2	1:A:295:TYR:CD1	2.37	0.42
1:A:507:ALA:O	1:A:508:VAL:C	2.61	0.42
1:A:733:MET:HE1	1:A:746:ALA:CB	2.49	0.42
1:A:964:LEU:O	1:A:964:LEU:HD23	2.19	0.42
1:A:992:LEU:HG	1:A:993:GLU:H	1.83	0.42
1:A:13:LEU:HD23	1:A:222:ILE:HD12	2.01	0.42
1:A:73:PHE:HA	1:A:91:PRO:CG	2.48	0.42
1:A:247:THR:CG2	1:A:250:GLN:CD	2.87	0.42
1:A:423:SER:O	1:A:446:THR:HG21	2.20	0.42
1:A:720:MET:HB3	1:A:738:ASP:OD1	2.20	0.42
1:A:963:ASP:C	1:A:963:ASP:OD1	2.61	0.42
1:A:983:ILE:O	1:A:987:ILE:HG12	2.18	0.42
1:A:1:MET:O	1:A:2:GLU:CB	2.64	0.42
1:A:7:LYS:HB2	1:A:8:SER:H	1.56	0.42
1:A:382:PHE:N	1:A:382:PHE:CD1	2.87	0.42
1:A:441:THR:CA	1:A:599:MET:HE1	2.44	0.42
1:A:880:HIS:HA	1:A:884:GLU:CB	2.49	0.42
1:A:459:VAL:HG23	1:A:462:LEU:HD12	2.01	0.42
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.50	0.42
1:A:877:THR:HG23	1:A:888:CYS:HB2	2.00	0.42
1:A:20:GLU:HG3	1:A:166:LEU:HD13	2.01	0.42
1:A:50:TRP:CH2	1:A:54:ILE:HD11	2.54	0.42
1:A:76:ALA:HB1	1:A:88:PHE:H	1.84	0.42
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.84	0.42
1:A:786:ALA:O	1:A:897:MET:HG2	2.19	0.42
1:A:950:VAL:CG1	1:A:951:ASP:N	2.48	0.42
1:A:497:TYR:HD1	1:A:512:MET:HE2	1.85	0.42
1:A:778:THR:HG23	1:A:779:ALA:N	2.33	0.42
1:A:635:ILE:O	1:A:639:ILE:HG12	2.20	0.42
1:A:340:GLU:C	1:A:342:LEU:H	2.27	0.42
1:A:379:LEU:HD12	1:A:379:LEU:N	2.35	0.42
1:A:88:PHE:CA	1:A:91:PRO:HD2	2.50	0.42
1:A:748:GLU:CA	1:A:817:MET:HE3	2.38	0.42
1:A:778:THR:CG2	1:A:779:ALA:N	2.82	0.42
1:A:326:MET:HE1	1:A:339:VAL:HG13	2.01	0.41
1:A:411:VAL:CG2	1:A:454:VAL:HG11	2.47	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ARG:HG3	1:A:535:VAL:N	2.35	0.41
1:A:336:LEU:N	1:A:337:PRO:CD	2.83	0.41
1:A:490:ASP:CG	1:A:491:ARG:N	2.79	0.41
1:A:322:GLY:O	1:A:323:THR:C	2.63	0.41
1:A:363:VAL:HG21	1:A:448:LEU:HD22	2.03	0.41
4:A:997:OTK:C31	4:A:997:OTK:C4	2.98	0.41
1:A:180:LEU:HG	1:A:180:LEU:O	2.21	0.41
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.87	0.41
1:A:870:LEU:HD12	1:A:870:LEU:C	2.45	0.41
1:A:893:ALA:HA	1:A:894:PRO:HD3	1.83	0.41
1:A:828:LEU:HA	1:A:828:LEU:HD23	1.82	0.41
1:A:680:GLU:OE2	1:A:682:SER:CB	2.68	0.41
1:A:840:ILE:HD13	1:A:980:LEU:HD23	2.02	0.41
1:A:898:THR:HG22	1:A:959:LEU:CD2	2.51	0.41
1:A:857:MET:O	1:A:859:ALA:N	2.46	0.41
1:A:909:MET:HE1	1:A:940:SER:HB2	2.02	0.41
1:A:77:TRP:CE3	1:A:78:PHE:N	2.88	0.41
1:A:643:GLY:H	1:A:646:GLU:HB3	1.86	0.41
1:A:881:PRO:HG2	1:A:882:HIS:H	1.86	0.41
1:A:7:LYS:HA	1:A:7:LYS:HD3	1.66	0.41
1:A:174:ARG:HB2	1:A:216:ALA:HB3	2.03	0.41
1:A:228:VAL:O	1:A:228:VAL:CG1	2.67	0.41
1:A:793:LEU:O	1:A:794:TRP:C	2.63	0.41
1:A:86:THR:O	1:A:86:THR:HG22	2.20	0.41
1:A:109:GLU:C	1:A:109:GLU:CD	2.88	0.41
1:A:577:VAL:HG23	1:A:583:ARG:HE	1.85	0.41
1:A:795:VAL:HA	1:A:799:THR:OG1	2.20	0.41
1:A:879:ASP:C	1:A:881:PRO:CD	2.91	0.41
1:A:880:HIS:CE1	1:A:881:PRO:HD3	2.56	0.41
1:A:244:GLN:OE1	1:A:712:LYS:HG2	2.21	0.40
1:A:361:MET:HE3	1:A:599:MET:HG3	2.02	0.40
1:A:367:PHE:HZ	1:A:545:ILE:HG23	1.86	0.40
1:A:466:GLU:O	1:A:467:ARG:C	2.64	0.40
1:A:538:THR:OG1	1:A:541:VAL:HG23	2.21	0.40
1:A:876:CYS:O	1:A:877:THR:C	2.64	0.40
1:A:320:ALA:O	1:A:324:ARG:HG3	2.21	0.40
1:A:840:ILE:HD13	1:A:980:LEU:CD2	2.50	0.40
1:A:909:MET:HE2	1:A:940:SER:HB2	2.03	0.40
1:A:864:GLY:O	1:A:865:VAL:CG2	2.70	0.40
1:A:898:THR:CG2	1:A:959:LEU:HA	2.51	0.40
1:A:428:ASN:HD22	1:A:428:ASN:H	1.68	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:PHE:HZ	1:A:596:VAL:HG13	1.87	0.40
1:A:739:ASN:O	1:A:742:THR:HB	2.22	0.40
4:A:997:OTK:O6	4:A:997:OTK:C1	2.69	0.40
4:A:997:OTK:H31A	4:A:997:OTK:O3	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%)	859 (87%)	87 (9%)	46 (5%)	2 12

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	78	PHE
1	A	80	GLU
1	A	245	ASP
1	A	453	ASN
1	A	677	ALA
1	A	863	PRO
1	A	990	ASN
1	A	992	LEU
1	A	42	PRO
1	A	43	ALA
1	A	120	LYS
1	A	509	GLY
1	A	581	SER
1	A	663	LEU
1	A	738	ASP
1	A	865	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	886	LEU
1	A	950	VAL
1	A	2	GLU
1	A	7	LYS
1	A	76	ALA
1	A	79	GLU
1	A	82	GLU
1	A	227	GLY
1	A	467	ARG
1	A	556	ARG
1	A	680	GLU
1	A	866	THR
1	A	961	ALA
1	A	3	ALA
1	A	122	TYR
1	A	353	THR
1	A	482	GLU
1	A	502	LYS
1	A	858	TYR
1	A	883	PHE
1	A	285	GLY
1	A	341	THR
1	A	397	LYS
1	A	951	ASP
1	A	974	SER
1	A	406	GLN
1	A	520	GLY
1	A	947	ILE
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%)	800 (95%)	40 (5%)	21	51

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	82	GLU
1	A	83	GLU
1	A	106	VAL
1	A	129	VAL
1	A	146	VAL
1	A	151	VAL
1	A	191	THR
1	A	247	THR
1	A	267	ILE
1	A	304	VAL
1	A	334	ARG
1	A	341	THR
1	A	355	THR
1	A	367	PHE
1	A	402	ILE
1	A	428	ASN
1	A	484	THR
1	A	514	VAL
1	A	521	VAL
1	A	533	THR
1	A	596	VAL
1	A	597	VAL
1	A	606	GLU
1	A	698	THR
1	A	716	ILE
1	A	783	LEU
1	A	788	ILE
1	A	790	VAL
1	A	805	THR
1	A	844	VAL
1	A	856	PHE
1	A	861	ASP
1	A	863	PRO
1	A	877	THR
1	A	887	ASP
1	A	890	ILE
1	A	929	VAL
1	A	937	ILE
1	A	962	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	868	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	OTK	A	997	-	35,38,38	0.90	1 (2%)	43,60,60	1.91	10 (23%)
5	PTY	A	998	-	23,23,49	1.77	2 (8%)	26,28,54	1.72	4 (15%)

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
4	OTK	A	997	-	-	2/22/84/84	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PTY	A	998	-	-	8/27/27/53	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	998	PTY	O30-C30	7.07	1.43	1.22
5	A	998	PTY	O4-C30	3.60	1.43	1.33
4	A	997	OTK	O9-C10	-2.70	1.43	1.48

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	998	PTY	O4-C30-O30	-6.07	108.44	123.63
4	A	997	OTK	O9-C32-C33	4.92	119.02	110.67
5	A	998	PTY	O30-C30-C31	-4.01	108.11	123.78
4	A	997	OTK	O3-C21-C22	3.59	120.87	111.46
4	A	997	OTK	O5-C6-C5	3.59	112.48	108.59
4	A	997	OTK	C6-O5-C12	-3.58	104.67	110.57
4	A	997	OTK	C3-O3-C21	-3.45	111.71	117.59
4	A	997	OTK	O7-C27-C28	3.33	118.67	111.48
4	A	997	OTK	O12-C12-C11	-3.26	124.98	128.28
4	A	997	OTK	C2-C1-C5	-2.81	99.98	103.85
5	A	998	PTY	C6-O7-C8	-2.57	111.64	117.80
5	A	998	PTY	O7-C8-C11	2.40	119.76	110.93
4	A	997	OTK	O3-C21-O4	-2.28	119.15	123.40
4	A	997	OTK	O5-C12-O12	2.14	124.36	121.60

There are no chirality outliers.

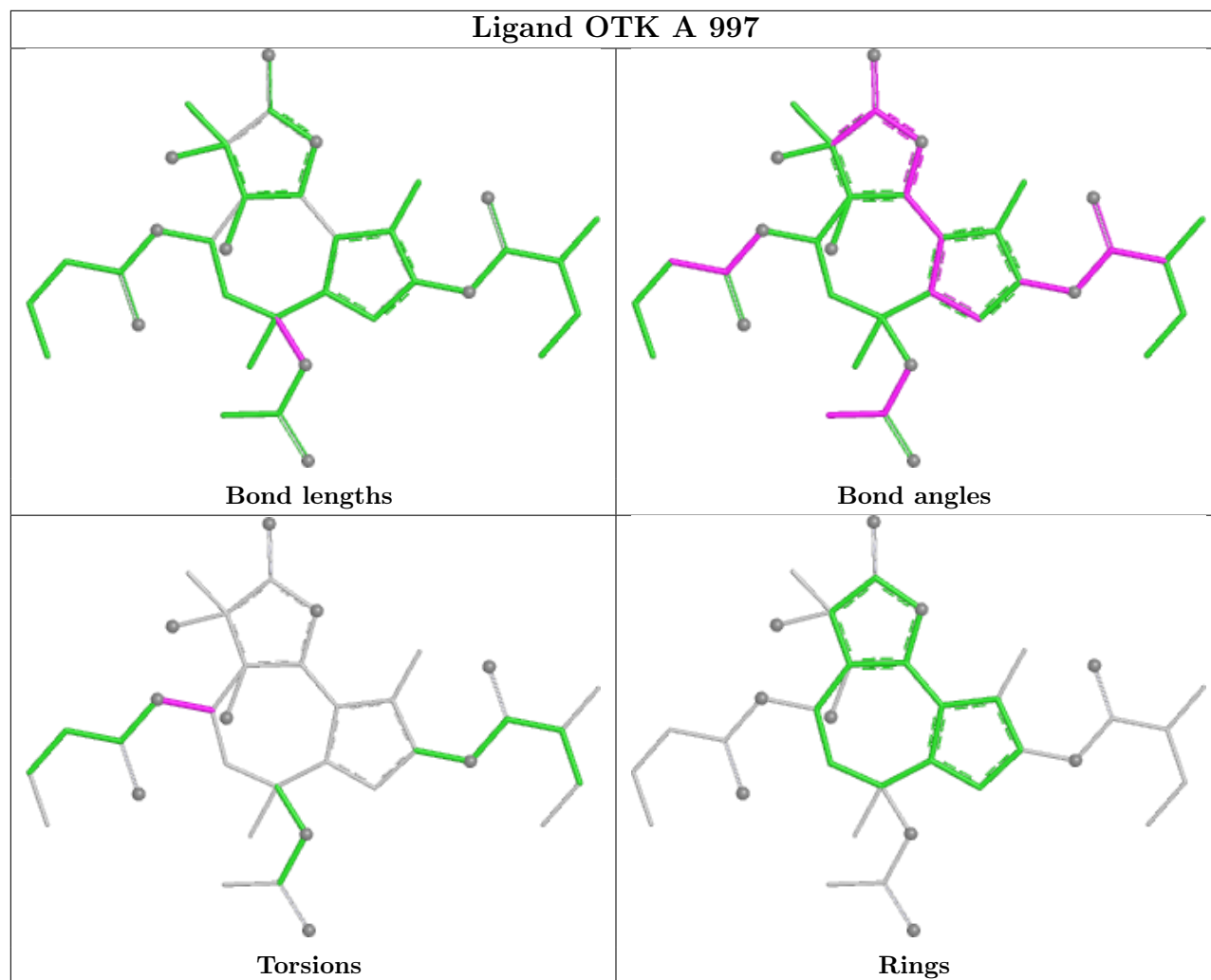All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	998	PTY	C3-O11-P1-O12
5	A	998	PTY	O30-C30-O4-C1
5	A	998	PTY	C31-C30-O4-C1
5	A	998	PTY	O4-C1-C6-O7
5	A	998	PTY	O4-C1-C6-C5
5	A	998	PTY	C3-O11-P1-O13
5	A	998	PTY	C3-O11-P1-O14
4	A	997	OTK	C9-C8-O7-C27
4	A	997	OTK	C7-C8-O7-C27
5	A	998	PTY	O4-C30-C31-C32

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	997	OTK	11	0
5	A	998	PTY	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand OTK A 997

Bond lengths

Bond angles

Torsions

Rings

Ligand PTY A 998

Bond lengths

Bond angles

Torsions

Rings
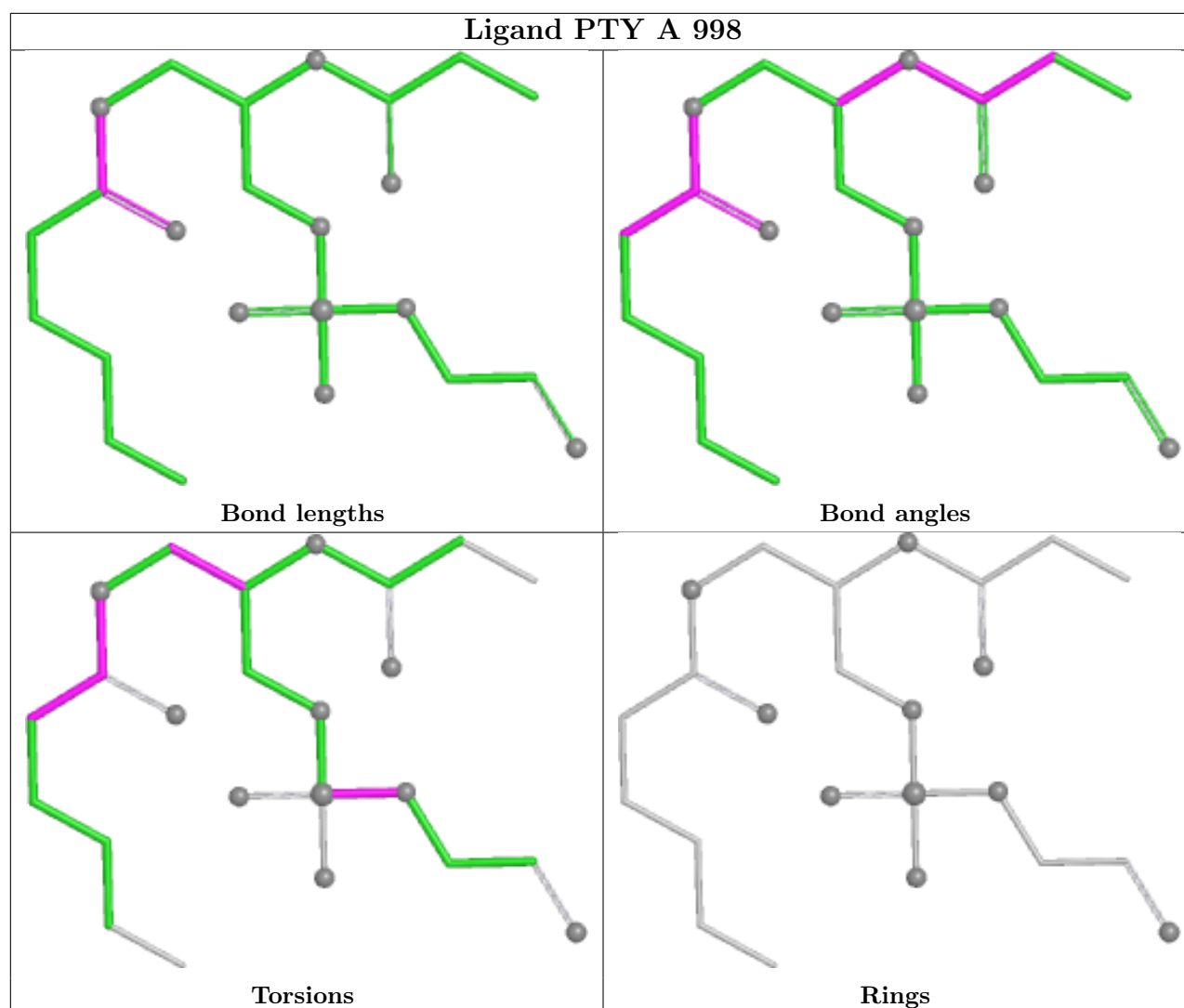
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	994/994 (100%)	-0.25	12 (1%)	76	60	55, 92, 130, 161	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	988	ALA	4.0
1	A	1	MET	3.2
1	A	733	MET	3.2
1	A	627	ASP	2.6
1	A	505	ARG	2.5
1	A	506	ALA	2.4
1	A	853	ALA	2.4
1	A	2	GLU	2.3
1	A	508	VAL	2.3
1	A	399	ASP	2.2
1	A	866	THR	2.1
1	A	884	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

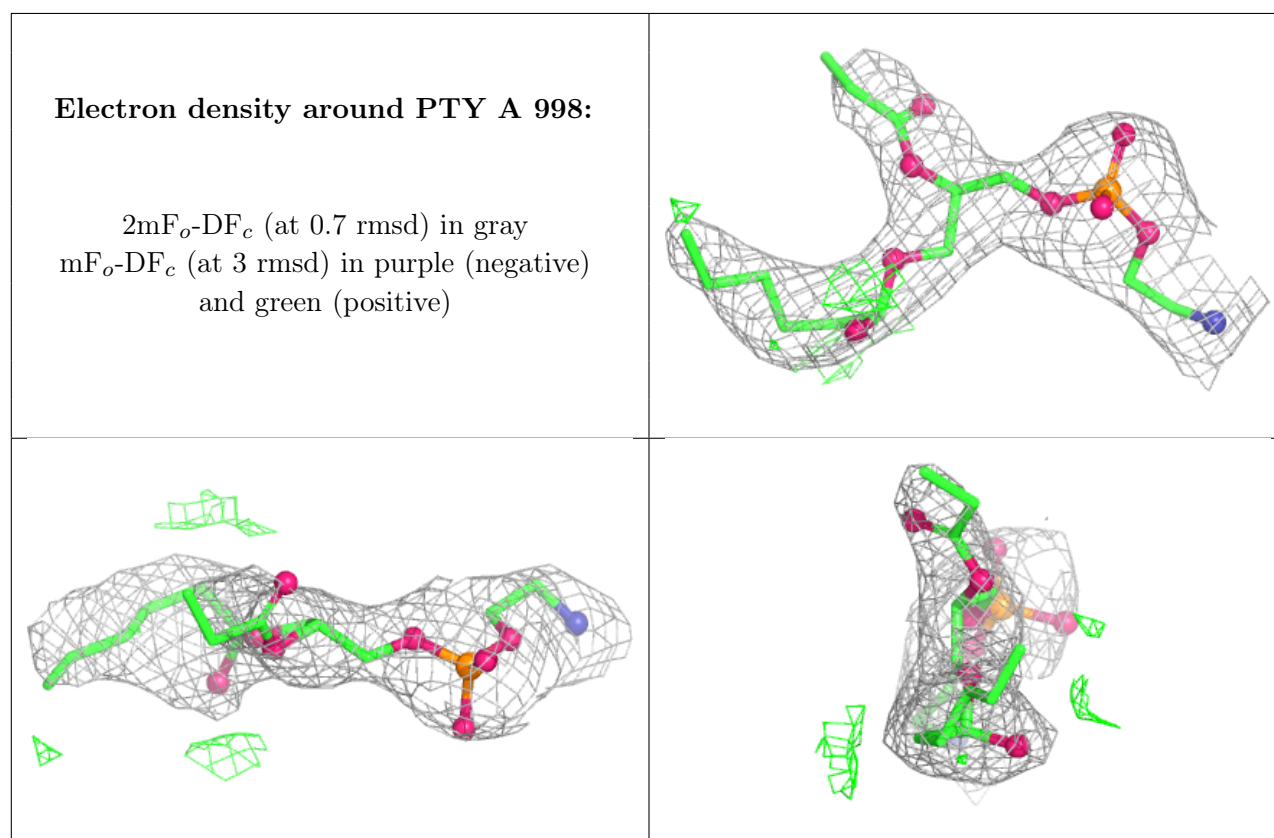## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.
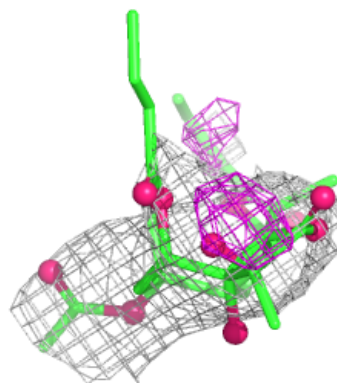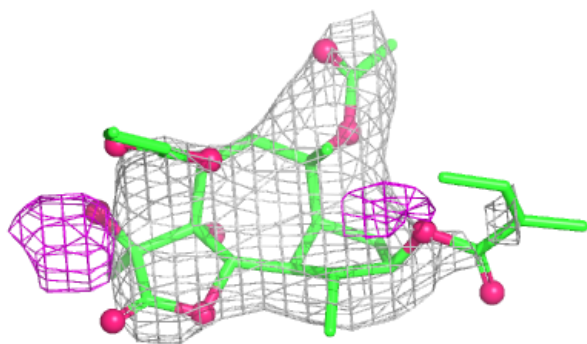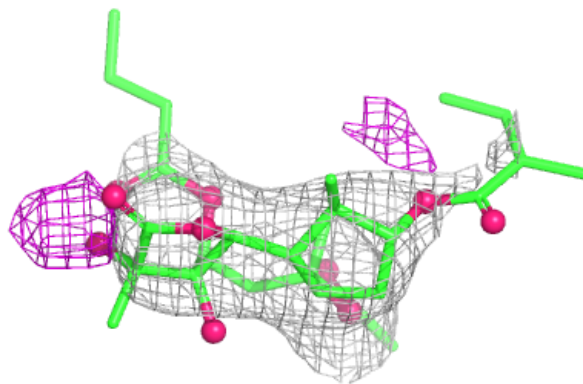
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PTY	A	998	24/50	0.77	0.16	113,123,130,132	0
4	OTK	A	997	36/36	0.84	0.19	136,143,146,147	0
3	MG	A	996	1/1	0.94	0.15	83,83,83,83	0
2	NA	A	995	1/1	0.95	0.08	46,46,46,46	0

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 998:

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

Electron density around OTK A 997:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.