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Table 4. Crystallographic details for (±)-(2*RS*,3*RS*,4*SR*,*PM*)/(2*RS*,3*RS*,4*RS*,*MP*)-*threo*-*N*-methyl-α-phenyl-2-piperidineacetic acid methyl ester (2) and (±)-(2*RS*,3*RS*,4*SR*,*PM*)-*threo*-*N*,*p*-dimethyl-α-phenyl-2-piperidineacetic acid methyl ester (5).

	data for **2**	data for **5**
Formula	$C_{15}H_{22}ClNO_2$	$C_{16}H_{24}ClNO_2$
FW, amu	283.79	297.81
Space group	$P2_1$	$C2/c$
a, Å	8.843(1)	19.274(2)
b, Å	18.406(4)	10.087(2)
c, Å	9.158(2)	16.363(2)
β, deg	90.33(2)	100.124(9)
V, Å^3	1490.6(5)	3131.6(7)
Z	4	8
F(000)	608	1280
ρ_{calcd}, g cm^{-3}	1.265	1.263
Linear absorption coefficient, mm^{-1}	2.250	2.165
Temperature, K	233	293
Crystal size, mm	0.24 x 0.32 x 0.42	0.06 x 0.28 x 0.52
Radiation	Graphite-monchromated Cu Kα $_{av}$	Graphite-monchromated Cu Kα $_{av}$
	(λ = 1.54178 Å)	(λ = 1.54178 Å)
Collection range	±*h*, ±*k*, ±*l*	±*h*, ±*k*, ±*l*
	$-9 \le h \le 9, -1 \le k \le 20, -9 \le l \le 5$	$-2 \le h \le 20, 1 \le k \le 11, -17 \le l \le 17$
2θ limits	$9.6° \le 2\theta \le 114.5°$	$9.6° \le 2\theta \le 114.5°$

Scan type	$2\theta/\omega$	$2\theta/\omega$
2θ scan range, deg	$1.5 + \Delta\alpha_1\alpha_2$	$1.5 + \Delta\alpha_1\alpha_2$
Data collected	2483	2585
Independent data/R_{int}	2483(0.02)	2139(0.03)
Unique data with $I_{net} \geq 2\sigma(I_{net})$	2126	1670
No. of variables/restraints	398/25	184
$R(F)^a$	0.036	0.062
${}_wR(F^2)^b$	0.125	0.162
Weighting factor, w	$[\sigma^2(F_{obs}{}^2) + (0.0915P)^2 + 0.5255P]^{-1}$ where $P = (F_{obs}{}^2 + 2F_{calc}{}^2)/3$ for both	$[\sigma^2(F_{obs}{}^2) + (0.0962P)^2 + 5.0610P]^{-1}$
Goodness of fit - all data[c]	1.07	1.06
Residual positive electron density, e/Å^3	0.34	0.26
Residual negative electron density, e/Å^3	–0.40	–0.52
Maximum shift/σ	0.051	0.005

Footnotes for Table

[a] The final discrepancy index $R(F)$ is defined as: $R(F) = (\Sigma_i \| \, |F_{obs}|_i - |F_{calc}|_i \, |)/(\Sigma_i |F_{obs}|_i)$;

[b] ${}_wR(F^2)$ was used, the ${}_wR(F)$ weighted value is defined as: ${}_wR(F) = \text{SQRT}\,[(\Sigma_i \{w_i (|F_{obs}|_i - |F_{calc}|_i)\}^2)/(\Sigma_i \{w_i (|F_{obs}|_i)\}^2)]$,

[c] Goodness of fit = $[\Sigma_i\{w_i(|F_{obs}|_i - |F_{calc}|_i\}^2)/(\text{no. of reflections} - \text{no. of parameters})]^{1/2}$.

Table 5. Fractional Coordinates, anisotropic equivalent (U_{eq}) and isotropic displacement parameters (U_{iso}) for non-hydrogen and selected hydrogen atoms of the (2*R*,3*R*,4*S*,*P*)/(2*R*,3*R*,4*R*,*M*)-enantiomers of molecules 1 and 2 of (±)-(2*RS*,3*RS*,4*SR*,*PM*)/(2*RS*,3*RS*,4*RS*,*MP*)-*threo*-*N*-methyl-α-phenyl-2-piperidineacetic acid methyl ester (2,2'); e.s.d.'s of last digit in parentheses.

	2 (Molecule-1)				**2'** (Molecule-2)			
	x	*y*	*z*	U_{aniso}/U_{iso}[a]	*x*	*y*	*z*	U_{aniso}/U_{iso}[a]
Atoms in common part								
Cl	0.9261(1)	0.85799(7)	0.6780(1)	0.0431(4)	0.4311(1)	0.42335(7)	0.8227(2)	0.0443(4)
O(1)	0.7840(4)	0.6803(3)	0.8001(5)	0.051(1)	0.2873(4)	0.6010(2)	0.6981(5)	0.049(1)
O(2)	0.8546(4)	0.7472(2)	0.9931(4)	0.0378(9)	0.3575(4)	0.5334(2)	0.5059(4)	0.0401(9)
C(1)	0.7545(6)	0.7237(3)	0.8958(6)	0.033(1)	0.2567(6)	0.5574(3)	0.6056(6)	0.032(1)
C(2)	0.5995(6)	0.7555(3)	0.9195(6)	0.030(1)	0.1028(5)	0.5248(3)	0.5789(5)	0.028(1)
H(2)	0.6103(6)	0.8022(3)	0.9699(6)	0.036	0.1138(5)	0.4781(3)	0.5285(5)	0.033
C(3)	0.5180(6)	0.7682(3)	0.7716(6)	0.034(1)	0.0227(6)	0.5127(3)	0.7265(5)	0.032(1)
H(3)	0.5328(6)	0.7244(3)	0.7124(6)	0.041	0.0380(6)	0.5564(3)	0.7859(5)	0.038
N(4)	0.5917(5)	0.8306(3)	0.6914(4)	0.036(1)	0.0958(5)	0.4498(3)	0.8061(5)	0.037(1)
H(4)	0.701(7)	0.821(3)	0.698(6)	0.039	0.192(7)	0.460(4)	0.798(1)	0.041
C(10)	1.0066(6)	0.7190(4)	0.9777(8)	0.055(2)	0.5083(6)	0.5616(5)	0.5233(8)	0.056(2)
C(11)	0.5094(6)	0.7036(3)	1.0166(5)	0.031(1)	0.0105(5)	0.5776(3)	0.4821(5)	0.030(1)
C(12)	0.4405(6)	0.7302(3)	1.1417(6)	0.038(1)	–0.0594(6)	0.5512(3)	0.3562(6)	0.036(1)
C(13)	0.3494(7)	0.6848(4)	1.2251(6)	0.049(2)	–0.1515(7)	0.5975(4)	0.2753(7)	0.050(2)
C(14)	0.3307(7)	0.6127(4)	1.1842(6)	0.050(2)	–0.1721(7)	0.6684(4)	0.3154(7)	0.049(2)
C(15)	0.4010(7)	0.5861(3)	1.0632(7)	0.044(1)	–0.0973(7)	0.6950(3)	0.4384(6)	0.044(1)
C(16)	0.4923(6)	0.6318(3)	0.9789(6)	0.035(1)	–0.0071(6)	0.6497(3)	0.5203(6)	0.036(1)
Atoms unique to A molecule, (2*RS*,3*RS*,4*SR*,*PM*), occupancy factor 0.710(7)								
C(5A)	0.548(2)	0.9036(8)	0.748(2)	0.043(4)	0.055(2)	0.3759(6)	0.748(2)	0.041(3)

C(6A)	0.3838(8)	0.9149(5)	0.765(1)	0.045(2)	–0.1116(9)	0.3662(5)	0.733(1)	0.050(2)
C(7A)	0.3095(8)	0.8536(5)	0.8524(9)	0.042(2)	–0.1878(8)	0.4260(5)	0.6460(9)	0.045(2)
C(8A)	0.349(1)	0.780(2)	0.784(3)	0.05(1)	–0.147(1)	0.499(1)	0.717(2)	0.047(9)
C(9A)	0.560(2)	0.826(3)	0.530(2)	0.059(8)	0.061(2)	0.457(2)	0.968(2)	0.061(8)
Atoms unique to B molecule, (*2RS,3RS,4RS,MP*), occupancy factor 0.290(7)								
C(5B)	0.545(4)	0.832(5)	0.536(3)	0.04(2)	0.058(3)	0.444(3)	0.9621(3)	0.026(9)
C(6B)	0.378(2)	0.844(1)	0.529(3)	0.059(6)	–0.111(2)	0.443(1)	0.972(1)	0.036(4)
C(7B)	0.297(3)	0.785(2)	0.616(3)	0.069(7)	–0.190(2)	0.503(1)	0.886(2)	0.043(5)
C(8B)	0.348(3)	0.779(4)	0.775(4)	0.04(3)	–0.147(3)	0.507(4)	0.726(4)	0.03(1)
C(9B)	0.572(5)	0.903(2)	0.772(5)	0.03(1)	0.077(4)	0.381(2)	0.712(3)	0.04(1)

Footnote for Table:

[a] U_{eq} is defined as one third the trace of the orthogonalized U_{ij} tensor. Anisotropic equivalent (U_{eq}) displacement parameters given for all non-hydrogen atoms in common part and for those unique to molecule A; U_{iso} isotropic displacement parameters for all non-hydrogen atoms unique to molecule B and for H(2),H(3), and H(4).

Table 6. Fractional Coordinates, isotropic displacement parameters (U_{iso}) for hydrogen atoms in the (2*R*,3*R*,4*S*,*P*)/(2*R*,3*R*,4*R*,*M*)-enantiomers of molecules 1 and 2 of (±)-(2*RS*,3*RS*,4*SR*,*PM*)/(2*RS*,3*RS*,4*RS*,*MP*)-*threo*-*N*-methyl-α-phenyl-2-piperidineacetic acid methyl ester (2,2'); e.s.d.'s of last digit in parentheses.[a]

	2 (Molecule-1)				**2'** (Molecule-2)			
	x	*y*	*z*	U_{iso}	*x*	*y*	*z*	U_{iso}
Atoms in common part								
H(2)	0.6103(6)	0.8022(3)	0.9699(6)	0.036	0.1138(5)	0.4781(3)	0.5285(5)	0.033
H(3)	0.5328(6)	0.7244(3)	0.7124(6)	0.041	0.0380(6)	0.5564(3)	0.7859(5)	0.038
H(4)	0.701(7)	0.821(3)	0.698(6)	0.039	0.192(7)	0.460(4)	0.798(1)	0.041
H(101)	1.0703(6)	0.7390(4)	1.0527(8)	0.083	0.5721(6)	0.5419(5)	0.4485(8)	0.083
H(102)	1.0048(6)	0.6670(4)	0.9863(8)	0.083	0.5062(6)	0.6136(5)	0.5154(8)	0.083
H(103)	1.0454(6)	0.7322(4)	0.8837(8)	0.083	0.5473(6)	0.5480(5)	0.6175(8)	0.083
H(12)	0.4553(6)	0.7782(3)	1.1697(6)	0.046	-0.0446(6)	0.5034(3)	0.3266(6)	0.043
H(13)	0.3013(7)	0.7026(4)	1.3077(6)	0.059	-0.2002(7)	0.5799(4)	0.1922(7)	0.061
H(14)	0.2696(7)	0.5824(4)	1.2396(6)	0.060	-0.2355(7)	0.6985(4)	0.2611(7)	0.059
H(15)	0.3884(7)	0.5377(3)	1.0368(7)	0.053	-0.1083(7)	0.7434(3)	0.4651(6)	0.052
H(16)	0.5414(6)	0.6136(3)	0.8972(6)	0.042	0.0426(6)	0.6678(3)	0.6023(6)	0.044
Atoms unique to molecule A, (2*RS*,3*RS*,4*SR*,*PM*), occupancy factor 0.710(7)								
H(51A)	0.586(2)	0.9403(8)	0.682(2)	0.052	0.095(2)	0.3391(6)	0.813(2)	0.050
H(52A)	0.597(2)	0.9109(8)	0.842(2)	0.052	0.102(2)	0.3693(6)	0.653(2)	0.050
H(61A)	0.3668(8)	0.9607(5)	0.815(1)	0.054	-0.1317(9)	0.3200(5)	0.686(1)	0.060
H(62A)	0.3366(8)	0.9179(5)	0.670(1)	0.054	-0.1558(9)	0.3645(5)	0.830(1)	0.060
H(71A)	0.3449(8)	0.8549(5)	0.9528(9)	0.050	-0.1536(8)	0.4249(5)	0.5455(9)	0.054
H(72A)	0.2006(8)	0.8601(5)	0.8523(9)	0.050	-0.2966(8)	0.4193(5)	0.6464(9)	0.054
H(81A)	0.304(1)	0.777(2)	0.688(3)	0.055	-0.189(1)	0.500(1)	0.814(2)	0.056
H(82A)	0.306(1)	0.742(2)	0.843(3)	0.055	-0.193(1)	0.538(1)	0.660(2)	0.056

H(91A)	0.588(2)	0.779(3)	0.495(2)	0.088	0.089(2)	0.505(2)	1.0000(2)	0.092
H(92A)	0.454(2)	0.834(3)	0.513(2)	0.088	-0.045(2)	0.450(2)	0.983(2)	0.092
H(93A)	0.617(2)	0.863(3)	0.481(2)	0.088	0.118(2)	0.422(2)	1.022(2)	0.092
Atoms unique to molecule B, (*2RS,3RS,4RS,MP*), occupancy factor 0.290(7)								
H(51B)	0.596(4)	0.872(5)	0.486(3)	0.051	0.101(3)	0.400(3)	1.004(3)	0.032
H(52B)	0.571(4)	0.787(5)	0.489(3)	0.051	0.099(3)	0.4844(3)	1.016(3)	0.032
H(61B)	0.354(2)	0.891(1)	0.568(3)	0.070	-0.147(2)	0.396(1)	0.936(2)	0.044
H(62B)	0.345(2)	0.842(1)	0.428(3)	0.070	-0.140(2)	0.447(1)	1.074(2)	0.044
H(71B)	0.189(3)	0.795(2)	0.614(3)	0.083	-0.167(2)	0.549(1)	0.932(2)	0.051
H(72B)	0.313(3)	0.739(2)	0.569(3)	0.083	-0.298(2)	0.496(1)	0.892(2)	0.051
H(81B)	0.299(3)	0.738(4)	0.822(4)	0.049	-0.180(3)	0.464(4)	0.674(4)	0.031
H(82B)	0.324(3)	0.823(4)	0.828(4)	0.049	-0.192(3)	0.550(4)	0.680(4)	0.031
H(91B)	0.605(5)	0.897(2)	0.871(5)	0.046	0.104(4)	0.391(2)	0.613(3)	0.054
H(92B)	0.632(5)	0.939(2)	0.725(5)	0.046	0.141(4)	0.343(2)	0.750(3)	0.054
H(93B)	0.468(5)	0.917(2)	0.770(5)	0.046	-0.027(4)	0.365(2)	0.715(3)	0.054

Table 7. Fractional Coordinates, anisotropic equivalent (U_{eq}) [for non-hydrogen atoms] and isotropic (U_{iso}) [for selected hydrogen atoms] displacement parameters of the (2*R*,3*R*,4*S*,*P*)-enantiomer of (±)-(2*RS*,3*RS*,4*SR*,*PM*)-*threo*-*N*,*p*-dimethyl-α-phenyl-2-piperidineacetic acid methyl ester (5); e.s.d.'s of last digit in parentheses.

Atom	*x*	*y*	*z*	U_{aniso}/U_{iso}[a]
Cl	0.39579(6)	0.1586(1)	0.63565(6)	0.0530(4)
O(1)	0.2331(2)	0.2943(3)	0.6716(2)	0.0521(8)
O(2)	0.2149(1)	0.0796(3)	0.6435(2)	0.0479(8)
C(1)	0.2322(2)	0.1809(4)	0.6938(2)	0.0350(9)
C(2)	0.2467(2)	0.1394(4)	0.7842(2)	0.0355(9)
H(2)	0.2619(2)	0.0466(4)	0.7871(2)	0.039
C(3)	0.3047(2)	0.2225(4)	0.8353(2)	0.040(1)
H(3)	0.2942(2)	0.3160(4)	0.8223(2)	0.044
N(4)	0.3757(2)	0.1917(3)	0.8121(2)	0.0393(8)
H(4)	0.373(2)	0.183(4)	0.759(3)	0.043
C(5)	0.4070(2)	0.0618(4)	0.8444(3)	0.053(1)
C(6)	0.4088(3)	0.0483(5)	0.9371(3)	0.062(1)
C(7)	0.3364(3)	0.0718(5)	0.9586(3)	0.060(1)
C(8)	0.3100(2)	0.2045(5)	0.9289(3)	0.052(1)
C(9)	0.4252(2)	0.3028(5)	0.8361(3)	0.055(1)
C(10)	0.2010(3)	0.1162(6)	0.5543(3)	0.066(2)
C(11)	0.1768(2)	0.1483(4)	0.8157(2)	0.0327(9)
C(12)	0.1457(2)	0.0360(4)	0.8396(2)	0.039(1)
C(13)	0.0809(2)	0.0419(4)	0.8653(3)	0.044(1)
C(14)	0.0458(2)	0.1609(4)	0.8679(3)	0.042(1)
C(15)	0.0781(2)	0.2741(4)	0.8453(3)	0.044(1)
C(16)	0.1427(2)	0.2686(4)	0.8195(2)	0.041(1)

C(17)	–0.0255(2)	0.1670(5)	0.8942(4)	0.068(1)

Footnote for table: [a] U_{eq} is defined as one third the trace of the orthogonalized U_{ij} tensor. U_{iso} given for H(2),H(3), and H(4) only.

Table 8. Fractional Coordinates, isotropic displacement parameters (U_{iso}) for hydrogen atoms in the (2*R*,3*R*,4*S*,*P*)-enantiomer of (±)-(2*RS*,3*RS*,4*SR*,*PM*)-*threo*-*N*,*p*-dimethyl-α-phenyl-2-piperidineacetic acid methyl ester (5); e.s.d.'s of last digit in parentheses.

Atom	*x*	*y*	*z*	U_{iso}
H(2)	0.2619(2)	0.0466(4)	0.7871(2)	0.039
H(3)	0.2942(2)	0.3160(4)	0.8223(2)	0.044
H(4)	0.373(2)	0.183(4)	0.759(3)	0.043
H(51)	0.4545(2)	0.0548(4)	0.8330(3)	0.059
H(52)	0.3794(2)	-0.0102(4)	0.8158(3)	0.059
H(61)	0.4418(3)	0.1120(5)	0.9665(3)	0.068
H(62)	0.4249(3)	-0.0398(5)	0.9550(3)	0.068
H(71)	0.3040(3)	0.0041(5)	0.9328(3)	0.066
H(72)	0.3390(3)	0.0662(5)	1.0182(3)	0.066
H(81)	0.3413(2)	0.2717(5)	0.9573(3)	0.057
H(82)	0.2638(2)	0.2181(5)	0.9433(3)	0.057
H(91)	0.4037(2)	0.3843(5)	0.8145(3)	0.071
H(92)	0.4675(2)	0.2881(5)	0.8138(3)	0.071
H(93)	0.4367(2)	0.3080(5)	0.8955(3)	0.071
H(101)	0.1887(3)	0.0382(6)	0.5213(3)	0.086
H(102)	0.2425(3)	0.1556(6)	0.5397(3)	0.086
H(103)	0.1628(3)	0.1785(6)	0.5442(3)	0.086
H(12)	0.1683(2)	-0.0453(4)	0.8386(2)	0.043
H(13)	0.0607(2)	-0.0356(4)	0.8810(3)	0.049
H(15)	0.0559(2)	0.3556(4)	0.8474(3)	0.048
H(16)	0.1633(2)	0.3462(4)	0.8047(2)	0.045
H(171)	-0.0417(2)	0.2572(5)	0.8922(4)	0.088
H(172)	-0.0218(2)	0.1337(5)	0.9498(4)	0.088
H(173)	-0.0585(2)	0.1138(5)	0.8572(4)	0.088

Table 9. Bond lengths in molecules 1 and 2 of (±)-(2*RS*,3*RS*,4*SR*,*PM*)/(2*RS*,3*RS*,4*RS*,*MP*)-*threo*-*N*-methyl-α-phenyl-2-piperidineacetic acid methyl ester (2,2') and (±)-(2*RS*,3*RS*,4*SR*,*PM*)-*threo*-*N*,*p*-dimethyl-α-phenyl-2-piperidineacetic acid methyl ester (5).[a]

Bond (Å)	**2** (molecule 1)	**2'** (molecule 2)	**5**	Bond (Å)	**2** (molecule 1)	**2'** (molecule 2)	**5**
Common part							
O(1)–C(1)	1.216(7)	1.196(7)	1.201(5)	C(11)–C(12)	1.389(8)	1.393(8)	1.371(5)
O(2)–C(1)	1.325(6)	1.353(6)	1.318(4)	C(11)–C(16)	1.373(8)	1.383(8)	1.388(5)
O(2)–C(10)	1.448(7)	1.439(7)	1.482(5)	C(12)–C(13)	1.393(9)	1.390(9)	1.386(5)
C(1)–C(2)	1.507(7)	1.506(7)	1.515(5)	C(13)–C(14)	1.387(10)	1.369(10)	1.382(6)
C(2)–C(3)	1.549(7)	1.546(7)	1.525(5)	C(14)–C(15)	1.365(9)	1.391(9)	1.381(6)
C(2)–C(11)	1.532(7)	1.545(7)	1.526(5)	C(14)–C(17)	n.a.[b]	n.a.[b]	1.512(6)
C(3)–N(4)	1.513(7)	1.511(7)	1.514(5)	C(15)–C(16)	1.401(8)	1.373(8)	1.384(6)
A Molecule, (2*RS*,3*RS*,4*SR*,*PM*), occupancy factor 0.710(7)							
C(3)–C(8A)	1.516(12)	1.520(12)	1.527(5)	C(5A)–C(6A)	1.48(2)	1.491(15)	1.517(7)
N(4)–C(5A)	1.491(13)	1.503(11)	1.500(5)	C(6A)–C(7A)	1.531(11)	1.515(11	1.516(7)
N(4)–C(9A)	1.502(14)	1.52(2)	1.480(5)	C(7A)–C(8A)	1.53(3)	1.53(3)	1.483(7)
B Molecule, (2*RS*,3*RS*,4*RS*,*MP*), occupancy factor 0.290(7)							
C(3)–C(8B)	1.51(2)	1.50(2)		C(5B)–C(6B)	1.49(3)	1.50(3)	
N(4)–C(5B)	1.48(3)	1.48(3)		C(6B)–C(7B)	1.53(2)	1.53(2)	
N(4)–C(9B)	1.53(3)	1.54(2)		C(7B)–C(8B)	1.52(3)	1.52(3)	

Footnote for Table:

[a] Atom descriptors for **5** have the letter "A" omitted. [b] Not applicable.

Table 10. Bond angles in molecules 1 and 2 of (±)-(2*RS*,3*RS*,4*SR*,*PM*)/(2*RS*,3*RS*,4*RS*,*MP*)-*threo*-*N*-methyl-α-phenyl-2-piperidineacetic acid methyl ester (2,2') and (±)-(2*RS*,3*RS*,4*SR*,*PM*)-*threo*-*N*,*p*-dimethyl-α-phenyl-2-piperidineacetic acid methyl ester (5).[a]

Bond angles (°)	**2** (molecule 1)	**2'** (molecule 2)	**5**	Bond angles (°)	**2** (molecule 1)	**2'** (molecule 2)	**5**
Common part							
O(1)–C(1)–O(2)	123.6(5)	123.3(5)	124.4(4)	C(12)–C(11)–C(16)	119.9(5)	119.6(5)	118.3(3)
O(2)–C(1)–C(2)	112.4(4)	111.0(4)	112.3(3)	C(11)–C(12)–C(13)	119.9(6)	118.9(5)	120.9(4)
C(1)–O(2)–C(10)	115.8(5)	114.9(5)	113.8(3)	C(12)–C(13)–C(14)	119.6(6)	121.3(6)	121.2(4)
C(1)–C(2)–C(3)	110.6(4)	109.5(4)	112.0(3)	C(13)–C(14)–C(15)	120.5(6)	119.3(6)	117.6(4)
C(1)–C(2)–C(11)	108.6(4)	108.4(4)	107.0(3)	C(13)–C(14)–C(17)	n.a.[b]	n.a.[b]	121.2(4)
C(3)–C(2)–C(11)	111.1(4)	110.4(4)	112.9(3)	C(14)–C(15)–C(16)	119.9(6)	120.1(6)	121.3(4)
N(4)–C(3)–C(2)	109.8(4)	109.6(4)	111.0(3)	C(11)–C(16)–C(15)	120.1(5)	120.7(5)	120.5(4)
C(2)–C(11)–C(12)	119.4(5)	119.1(5)	120.3(3)				
A Molecule, (2*RS*,3*RS*,4*SR*,*PM*), occupancy factor 0.710(7)							
C(2)–C(3)–C(8A)	114.2(9)	115.3(9)	113.4(3)	N(4)–C(5A)–C(6A)	115.0(11)	112.0(9)	111.6(4)
N(4)–C(3)–C(8A)	110.6(10)	108.5(10)	108.9(3)	C(5A)–C(6A)–C(7A)	112.2(9)	113.4(8)	110.9(4)
C(3)–N(4)–C(5A)	113.7(8)	115.0(6)	114.6(3)	C(6A)–C(7A)–C(8A)	109.7(10)	108.0(9)	110.0(4)
C(3)–N(4)–C(9A)	111.0(16)	108.3(11)	110.3(3)	C(3)–C(8A)–C(7A)	112.8(15)	113.9(14)	113.2(4)
C(5A)–N(4)–C(9A)	109.8(18)	112.2(13)	111.5(3)				
B Molecule, (2*RS*,3*RS*,4*RS*,*MP*), occupancy factor 0.290(7)							
C(2)–C(3)–C(8B)	117.4(15)	118.0(14)		N(4)–C(5B)–C(6B)	108.6(24)	106.3(20)	
N(4)–C(3)–C(8B)	109.6(23)	112.1(23)		C(5B)–C(6B)–C(7B)	110.2(36)	114.4(25)	
C(3)–N(4)–C(5B)	111.4(33)	115.2(22)		C(6B)–C(7B)–C(8B)	114.4(30)	114.9(26)	
C(3)–N(4)–C(9B)	112.1(19)	108.5(14)		C(3)–C(8B)–C(7B)	106.3(24)	104.9(21)	

C(5B)–N(4)–C(9B)	114.3(38)	117.2(27)

Footnote for Table:

[a] Atom descriptors for **5** have the letter "A" omitted. [b] Not applicable.

Table 11. Torsion angles in (2*R*,3*R*,4*S*,*P*)/(2*R*,3*R*,4*R*,*M*)-enantiomers of molecules 1 and 2 (±)-(2*RS*,3*RS*,4*SR*,*PM*)/(2*RS*,3*RS*,4*RS*,*MP*)-*threo*-*N*-methyl-α-phenyl-2-piperidineacetic acid methyl ester (2,2'), and for (2*R*,3*R*,4*S*,*P*)-enantiomer of (±)-(2*RS*,3*RS*,4*SR*,*PM*)-*threo*-*N*,*p*-dimethyl-α-phenyl-2-piperidineacetic acid methyl ester (5).[a]

Torsion angles (°)	**2** (molecule 1)	**2'** (molecule 2)	**5**	Torsion angles (°)	**2** (molecule 1)	**2'** (molecule 2)	**5**
Common part							
O(1)–C(1)–O(2)–C(10)	1.4(8)	2.9(8)	4.2(5)	C(3)–C(2)–C(11)–C(16)	67.3(6)	66.7(6)	59.5(5)
C(2)–C(1)–O(2)–C(10)	–179.9(5)	–179.7(5)	–179.5(3)	C(2)–C(11)–C(12)–C(13)	175.4(5)	175.2(5)	–177.5(3)
O(1)–C(1)–C(2)–C(3)	–36.2(7)	–36.7(7)	–38.0(5)	C(16)–C(11)–C(12)–C(13)	–2.6(8)	–3.1(7)	1.4(6)
O(1)–C(1)–C(2)–C(11)	86.0(6)	83.9(6)	86.1(4)	C(2)–C(11)–C(16)–C(15)	–175.6(5)	–175.8(5)	177.6(3)
O(2)–C(1)–C(2)–C(3)	145.2(4)	146.1(4)	145.6(3)	C(12)–C(11)–C(16)–C(15)	2.4(7)	2.4(8)	–1.3(6)
O(2)–C(1)–C(2)–C(11)	–92.6(5)	–93.4(5)	–90.3(4)	C(11)–C(12)–C(13)–C(14)	1.4(9)	1.4(9)	–0.3(6)
C(1)–C(2)–C(3)–N(4)	–70.8(5)	–72.4(5)	–69.5(4)	C(12)–C(13)–C(14)–C(15)	0.1(10)	1.1(9)	–1.0(6)
C(11)–C(2)–C(3)–N(4)	168.5(4)	168.3(4)	169.7(3)	C(12)–C(13)–C(14)–C(17)	n.a.[b]	n.a.[b]	178.7(4)
C(1)–C(2)–C(11)–C(12)	127.5(5)	128.5(5)	114.7(4)	C(13)–C(14)–C(15)–C(16)	–0.4(9)	–1.7(9)	–1.1(6)
C(1)–C(2)–C(11)–C(16)	–54.5(6)	–53.3(6)	–64.1(4)	C(17)–C(14)–C(15)–C(16)	n.a.[b]	n.a.[b]	–178.6(4)
C(3)–C(2)–C(11)–C(12)	–110.7(5)	–111.5(5)	–121.6(4)	C(14)–C(15)–C(16)–C(11)	–0.9(8)	0.0(8)	0.1(6)
A Molecule, (2*RS*,3*RS*,4*SR*,*PM*), occupancy factor 0.710(7)							
C(1)–C(2)–C(3)–C(8A)	164.2(12)	164.8(11)	167.6(3)	N(4)–C(3)–C(8A)–C(7A)	–53.8(16)	–55.2(14)	–54.7(5)
C(11)–C(2)–C(3)–C(8A)	43.5(13)	45.5(12)	46.8(5)	C(3)–N(4)–C(5A)–C(6A)	–49.2(15)	–50.9(11)	–51.8(5)
C(2)–C(3)–N(4)–C(5A)	–77.7(8)	–75.7(8)	–74.7(4)	C(9A)–N(4)–C(5A)–C(6A)	75.8(18)	73.4(13)	74.4(5)
C(2)–C(3)–N(4)–C(9A)	157.9(12)	158.0(10)	158.5(3)	N(4)–C(5A)–C(6A)–C(7A)	50.9(16)	52.7(12)	53.5(5)
C(8A)–C(3)–N(4)–C(5A)	49.3(13)	51.0(12)	50.8(4)	C(5A)–C(6A)–C(7A)–C(8A)	–53.1(12)	–55.1(11)	–57.1(5)
C(8A)–C(3)–N(4)–C(9A)	–75.1(16)	–75.2(14)	–76.0(4)	C(6A)–C(7A)–C(8A)–C(3)	55.7(16)	57.4(14)	58.9(5)

C(2)–C(3)–C(8A)–C(7A)	70.7(16)	68.2(15)	69.4(5)

B Molecule, (*2RS,3RS,4RS,MP*), occupancy factor 0.290(7)

C(1)–C(2)–C(3)–C(8B)	163.1(31)	157.7(31)		N(4)–C(3)–C(8B)–C(7B)	57.5(42)	56.5(43)
C(11)–C(2)–C(3)–C(8B)	42.4(31)	38.4(32)		C(3)–N(4)–C(5B)–C(6B)	61.9(57)	54.5(39)
C(2)–C(3)–N(4)–C(5B)	165.3(23)	164.7(18)		C(9B)–N(4)–C(5B)–C(6B)	–66.4(61)	–75.1(40)
C(2)–C(3)–N(4)–C(9B)	–65.2(16)	–61.6(14)		N(4)–C(5B)–C(6B)–C(7B)	–55.8(61)	–49.7(42)
C(8B)–C(3)–N(4)–C(5B)	–64.3(31)	–62.4(29)		C(5B)–C(6B)–C(7B)–C(8B)	55.5(38)	54.3(32)
C(8B)–C(3)–N(4)–C(9B)	65.2(27)	71.4(27)		C(6B)–C(7B)–C(8B)–C(3)	–55.1(47)	–54.0(45)
C(2)–C(3)–C(8B)–C(7B)	–176.3(24)	–174.8(22)				

Footnote for Table:

[a] Atom descriptors for **5** have the letter "A" omitted. [b] Not applicable.

Table 12. Anisothermal parameters for (2*R*,3*R*,4*S*,*P*)-enantiomers of molecules 1 and 2 of (±)-(2*RS*,3*RS*,4*SR*,*PM*)/(2*RS*,3*RS*,4*RS*,*MP*)-*threo*-*N*-methyl-α-phenyl-2-piperidineacetic acid methyl ester (2,2').[a]

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Atoms in common part, **2** (Molecule 1)						
C*l*1	0.0388(7)	0.0472(8)	0.0432(7)	0.0061(6)	–0.0024(5)	–0.0100(6)
O(1)	0.037(2)	0.060(3)	0.056(3)	–0.015(2)	0.007(2)	–0.004(2)
O(2)	0.028(2)	0.049(2)	0.037(2)	–0.004(2)	–0.001(2)	–0.001(2)
C(1)	0.033(3)	0.036(3)	0.030(3)	0.004(2)	0.002(2)	–0.007(2)
C(2)	0.031(3)	0.029(3)	0.030(3)	0.003(2)	–0.002(2)	-0.004(2)
C(3)	0.040(3)	0.031(3)	0.032(3)	0.007(2)	–0.005(2)	-0.006(2)
N(4)	0.037(2)	0.037(3)	0.033(2)	0.010(2)	0.002(2)	–0.005(2)
C(10)	0.029(3)	0.071(5)	0.065(4)	0.001(4)	–0.006(3)	0.005(3)
C(11)	0.029(3)	0.041(3)	0.024(2)	0.006(2)	–0.003(2)	0.000(2)
C(12)	0.040(3)	0.041(3)	0.033(3)	–0.002(2)	0.006(2)	0.000(3)
C(13)	0.047(4)	0.063(4)	0.038(3)	0.009(3)	0.015(3)	0.005(3)
C(14)	0.049(4)	0.058(4)	0.042(3)	0.022(3)	0.004(3)	–0.015(3)
C(15)	0.053(3)	0.035(3)	0.045(3)	0.009(3)	–0.001(3)	–0.011(3)
C(16)	0.038(3)	0.033(3)	0.034(3)	0.005(2)	0.000(2)	–0.006(2)
Atoms in common part, **2'** (Molecule 2)						
C*l*2	0.0401(7)	0.0474(8)	0.0454(7)	0.0050(6)	0.0019(5)	0.0108(6)
O(1')	0.042(2)	0.048(2)	0.058(3)	–0.019(2)	–0.008(2)	0.002(2)
O(2')	0.030(2)	0.053(2)	0.038(2)	–0.002(2)	0.006(2)	–0.003(2)
C(1')	0.033(3)	0.030(3)	0.034(3)	0.002(2)	–0.003(2)	0.005(2)
C(2')	0.028(3)	0.027(3)	0.028(3)	–0.003(2)	–0.001(2)	0.004(2)
C(3')	0.037(3)	0.032(3)	0.026(3)	–0.003(2)	0.000(2)	0.003(2)

N(4')	0.033(2)	0.043(3)	0.035(3)	0.007(2)	–0.002(2)	0.002(2)
C(10')	0.027(3)	0.076(5)	0.064(4)	0.001(4)	0.002(3)	–0.006(3)
C(11')	0.026(3)	0.032(3)	0.033(3)	0.002(2)	0.003(2)	0.000(2)
C(12')	0.038(3)	0.037(3)	0.032(3)	0.001(2)	–0.004(2)	0.001(2)
C(13')	0.051(4)	0.064(4)	0.036(3)	0.003(3)	–0.012(3)	–0.009(3)
C(14')	0.044(3)	0.051(4)	0.053(4)	0.023(3)	–0.001(3)	0.008(3)
C(15')	0.048(3)	0.037(3)	0.045(3)	0.008(3)	0.003(3)	0.007(3)
C(16')	0.042(3)	0.035(3)	0.032(3)	0.003(2)	–0.003(2)	0.002(2)
Atoms unique to molecule **2-A**, (2*RS*,3*RS*,4*SR*,*PM*), occupancy factor 0.710(7)						
C(5A)	0.039(8)	0.036(6)	0.055(9)	0.013(5)	–0.013(6)	-0.002(4)
C(6A)	0.035(4)	0.036(4)	0.065(5)	–0.003(4)	–0.010(4)	0.011(4)
C(7A)	0.020(3)	0.051(5)	0.055(5)	0.010(4)	–0.001(3)	0.010(4)
C(8A)	0.026(10)	0.052(15)	0.058(14)	0.023(7)	–0.012(4)	–0.015(5)
C(9A)	0.052(9)	0.089(18)	0.036(7)	0.017(6)	–0.002(4)	–0.001(8)
Atoms unique to molecule **2'-A**, (2*RS*,3*RS*,4*SR*,*PM*), occupancy factor 0.710(7)						
C(5A')	0.058(7)	0.029(6)	0.037(7)	0.011(4)	0.007(5)	–0.006(4)
C(6A')	0.045(5)	0.043(5)	0.063(5)	0.004(4)	0.007(4)	–0.010(4)
C(7A')	0.025(4)	0.057(6)	0.053(5)	0.008(4)	0.002(3)	–0.003(4)
C(8A')	0.035(7)	0.060(16)	0.046(8)	0.010(7)	0.012(4)	0.014(5)
C(9A')	0.068(9)	0.078(19)	0.037(7)	0.021(7)	0.008(4)	0.011(7)

Footnotes for table:

[a] Anisotropic temperature factors are of the form: $Temp = -2\pi^2(h^*h^*u_{11}^*astar^*astar + \text{---} + 2^*h^*k^*u_{12}^*astar^*bstar + \text{---})$

Table 13. Anisothermal parameters for (2*R*,3*R*,4*S*,*P*)-enantiomer of (±)-(2*RS*,3*RS*,4*SR*,*PM*)/(2*RS*,3*RS*,4*RS*,*MP*)-*threo*-*N*,*p*-dimethyl-α-phenyl-2-piperidineacetic acid methyl ester (5).[a]

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl	0.0460(6)	0.0687(8)	0.0456(6)	–0.0126(5)	0.0116(5)	–0.0028(5)
O(1)	0.060(2)	0.043(2)	0.053(2)	0.009(2)	0.010(2)	–0.001(2)
O(2)	0.053(2)	0.051(2)	0.040(2)	–0.008(1)	0.010(1)	–0.014(1)
C(1)	0.027(2)	0.041(3)	0.037(2)	–0.004(2)	0.006(2)	–0.005(2)
C(2)	0.031(2)	0.041(2)	0.033(2)	0.000(2)	0.002(2)	0.001(2)
C(3)	0.033(2)	0.045(2)	0.040(2)	–0.003(2)	0.004(2)	0.004(2)
N(4)	0.030(2)	0.051(2)	0.036(2)	–0.002(2)	0.004(1)	0.003(2)
C(5)	0.042(2)	0.054(3)	0.061(3)	–0.007(2)	0.001(2)	0.002(2)
C(6)	0.069(3)	0.048(3)	0.058(3)	0.004(2)	–0.016(2)	0.007(2)
C(7)	0.068(3)	0.073(3)	0.036(2)	–0.001(2)	0.002(2)	–0.021(3)
C(8)	0.042(2)	0.078(3)	0.036(2)	–0.010(2)	0.006(2)	–0.001(2)
C(9)	0.047(3)	0.056(3)	0.058(3)	–0.004(2)	0.000(2)	–0.010(2)
C(10)	0.066(3)	0.099(4)	0.032(2)	–0.004(3)	0.004(2)	–0.012(3)
C(11)	0.027(2)	0.041(2)	0.030(2)	–0.001(2)	0.003(2)	0.002(2)
C(12)	0.036(2)	0.033(2)	0.049(2)	–0.003(2)	0.008(2)	0.003(2)
C(13)	0.034(2)	0.041(2)	0.058(3)	–0.005(2)	0.011(2)	–0.011(2)
C(14)	0.027(2)	0.052(3)	0.049(2)	–0.012(2)	0.008(2)	–0.001(2)
C(15)	0.034(2)	0.044(2)	0.053(3)	–0.002(2)	0.003(2)	0.011(2)
C(16)	0.033(2)	0.042(2)	0.046(2)	0.009(2)	0.003(2)	–0.002(2)
C(17)	0.039(3)	0.076(4)	0.093(4)	–0.017(3)	0.023(3)	–0.002(2)

Footnotes for table:

[a] Anisotropic temperature factors are of the form: $Temp = -2\pi^2(h^*h^*u_{11}^*astar^*astar + \text{---} + 2^*h^*k^*u_{12}^*astar^*bstar + \text{---})$